รายงานฉบับสมบูรณ์ สัญญาที่ RTA/04/2542
ทุนเมธีวิจัยอาวุโส รุ่นที่ 4
ศาสตราจารย์ ดร.วิรุฬห์ สายคณิต
สนับสนุนทุนวิจัยโดย สำนักงานกองทุนสนับสนุนการวิจัย (สกว.)
ระยะเวลาโครงการตั้งแต่ 1 มิถุนายน 2542 – 30 พฤษภาคม 2545

โครงการ
"การเสริมกำลังให้ฟอรัมวิทยาศาสตร์ทฤษฎี เป็นศูนย์กลางวิทยาศาสตร์ทฤษฎีในประเทศไทย"

(Strengthening Forum for Theoretical Science (FTS) as the Center of Theoretical Science in Thailand)

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Content

กิตติกรรมประกาศ

ผม ศาสตราจารย์ ดร.วิรุฬห์ สายคณิต ผู้รับทุนเมธีวิจัยอาวุโส รุ่นที่ 4 หัวหน้าหน่วยวิจัยฟอรัมวิทยาศาสตร์ทฤษฎี ภาควิชาฟิสิกส์ คณะวิทยาศาสตร์ จุฬาลงกรณ์มหาวิทยาลัย และคณะผู้วิจัย ขอขอบคุณ สำนักงานกองทุนสนับสนุนการวิจัย (สกว.) ที่ได้ให้ทุนสนับสนุนดำเนินโครงการ "การเสริมกำลังให้ฟอรัมวิทยาศาสตร์ทฤษฎีเป็นศูนย์กลางวิทยาศาสตร์ทฤษฎีในประเทศไทย" (Strengthening Forum for Theoretical Science (FTS) as the Center of Theoretical Science in Thailand)

การดำเนินการโครงการนี้ ได้สำเร็จลุล่วงไปได้ด้วยดีด้วยการสนับสนุนจาก สกว. และความร่วมมือจากนักวิจัย ผู้ช่วยวิจัย และบุคคลต่าง ๆ ทั้งในประเทศและต่างประเทศ โดยสามารถผลิตผลงานวิจัยลงตีพิมพ์ในเอกสารทางวิชาการ และการเสนอผลงานในการประชุมทั้งภายในประเทศและต่างประเทศ ตลอดจนการสร้างนักวิจัยรุ่นใหม่ ๆ เพื่อรองรับการพัฒนาทางด้านวิทยาศาสตร์กายภาพและคณิตศาสตร์ในอนาคต

สุดท้ายนี้ คณะผู้วิจัยขอขอบพระคุณ สำนักงานกองทุนสนับสนุนการวิจัย (สกว.) ผู้ให้ทุนสนับสนุน และนักวิจัย ผู้ช่วยวิจัย และบุคลากรทุกท่าน ที่ทำให้โครงการนี้สำเร็จลุล่วงไปด้วยดี

บทคัดย่อ

ฟอรัมวิทยาศาสตร์ทฤษฎี (FTS) เป็นหน่วยงานขึ้นตรงกับจุฬาลงกรณ์มหาวิทยาลัย โดยมีวัตถุประสงค์ เพื่อรวบรวมนักวิจัยทางด้านการใช้คณิตศาสตร์ในการประยุกต์กับวิทยาศาสตร์ ฟอรัมฯ ได้รับการสนับสนุนจาก สำนักงานกองทุนสนับสนุนการวิจัย (สกว.) เป็นระยะที่สอง ต่อเนื่องทางด้านวิทยาศาสตร์กายภาพและคณิตศาสตร์ เพื่อให้มีศักยภาพในการวิจัยและเป็นเวทีเพื่อสร้างงานวิจัย ตลอดจนพัฒนาบุคลากรทั้งนักวิจัย ผู้ช่วยวิจัย นิสิตนักศึกษาในระดับปริญญาโทและเอก

ในระยะเวลา 3 ปีที่ผ่านมา ฟอรัมฯ มีผลงานตีพิมพ์ในต่างประเทศโดยได้ลงตีพิมพ์ในวารสารชั้นนำ อาทิ Rhys. Rev.3 บทความ ได้แก่ "Path Integral Derivation of Magnus Force", Phys. Rev. B60, 9299 (1999), 2) "Electronic transport properties of Sierpinski lattices", Phys. Rev. B60, 19, 13444 (1999) และ 3) "Effect of Random Well-Width Fluctuations on the Exciton Optical Absorption Spectrum in Single Quantum Wells", Phys. Rev. B62, 5079 (2000) นอกนั้นจะเป็น J. Phys. A จำนวน 1 บทความ ได้แก่ "Magnus Force and Hellmann-Feynman Force, path integral approach, J. Phys. A: Math Gen.34, 11301 (2001) และการเสนอต่อที่ประชุมนานาชาติ Proceedings จำนวน 5 บทความ

ตลอดระยะเวลา 3 ปี ฟอรัมฯ ได้ขยายขอบเขตการนำคณิตศาสตร์มาประยุกต์กับ Biology โดยได้จัดประชุมนานาชาติในหัวข้อเรื่อง "Biological Physics" ขึ้นในปี 2000 และจัดประชุมร่วมกับสมาคมฟิสิกส์ไทยในหัวข้อเรื่อง "Nanotechnology"

สำหรับการสร้างวิจัยนั้น ได้มีนักเรียนที่กำลังศึกษาอยู่ในระดับปริญญาเอกในโครงการจำนวน 6 คน และปริญญาโทจำนวน 10 คน โดยเป็นผู้ช่วยนักวิจัยในโครงการจำนวน 3 คน นอกจากนี้ ยังมี postdoc. จำนวน 1 คน และเป็นอาจารย์ที่ปรึกษาให้กับนิสิตปริญญาตรี จุฬาลงกรณ์มหาวิทยาลัย จำนวน 1 คน และโครงการพัฒนาอัจฉริยภาพทางวิทยาศาสตร์ซึ่งกำลังศึกษาอยู่ที่ มหาวิทยาลัยสงขลานครินทร์ จำนวน 1 คน โดยใน 3 ปีนี้ สามารถผลิตนักวิจัยออกไปเป็นบัณฑิตในระดับปริญญาโทจำนวน 9 คน และระดับปริญญาตรี จำนวน 1 คน

นอกจากนี้ ยังมีความร่วมมือกับสถาบันการศึกษาและวิจัยทั้งภายในประเทศและต่างประเทศ เพื่อทำงานวิจัยและแลกเปลี่ยนนักวิจัยระหว่างกัน โดยมีผลงานวิจัยในวารสารระดับนานาชาติ เช่น "On the Fourier Transform of the Diamond Kernel of Marcel Riesz", Applied Mathematics and Computation 101, 151 (1999), "On the Convolutions of the Diamond Kernel of Marcel Riesz", Applied Mathematics and Computation 114, 95 (2000), "On the Multiplicative Product on the Dirac-Delta Distribution on the Hyper-Surface", Computational Technologies, Vol.4, No.5 (1999), "On the Product of Ultra-Hyperbolic Operator Related to the Elastic Waves", Computational Technologies, Vol.4, No.5 (1999)

Summary of Research Activities

Forum for Theoretical Science (FTS) is a unit established by Chulalongkorn University with the main purpose of undertaking research in theoretical sciences and mathematics.

FTS has been receiving financial support from TRF for two consecutive periods from 1996 to 2002. The fund has enabled FTS to continue and stimulate research in various areas of sciences and mathematics. At the same time FTS has played an important role in training of many high potential research scientists.

For the last three years, FTS has published research papers in leading international journals viz. three papers in Phys. Rev: "Path Integral Derivation of Magnus Force", Phys. Rev. B60, 9299 (1999), "Electronic transport properties of Sierpinski lattices", Phys. Rev. B60, 19, 13444 (1999) and "Effect of Random Well-Width Fluctuations on the Exciton Optical Absorption Spectrum in Single Quantum Wells", Phys. Rev. B62, 5079 (2000); one paper in J. Phys.: "Magnus Force and Hellmann-Feynman Force, path integral approach, J. Phys. A: Math Gen.34, 11301 (2001). In addition, there are also 5 scientific papers presented at international conferences.

FTS has also expanded the areas of research interest to Biology and Nanotechnology by organizing an international workshop on Biological Physics in 2000 and co-organizing a meeting on Nanotechnology with Thai Institute of Physics in 2002.

For training of young research scientists, there are altogether 6 doctorate, 10 masterate and 2 undergraduate students doing research under the supervision of FTS staff; 3 research assistants and one post-doc. of these numbers, 9 masterate and 2 undergraduates have since graduated. Regarding collaboration with other universities and research institutes both locally and internationally, there have been many joint research activities and exchanges of visiting professors and scientists. Several research results were published in international journals e.g. "On the Fourier Transform of the Diamond Kernel of Marcel Riesz", Applied Mathematics and Computation 101, 151 (1999), "On the Convolutions of the Diamond Kernel of Marcel Riesz", Applied Mathematics and Computation 114, 95 (2000), "On the Multiplicative Product on the Dirac-Delta Distribution on the Hyper-Surface", Computational Technologies, Vol.4, No.5 (1999), "On the Product of Ultra-Hyperbolic Operator Related to the Elastic Waves", Computational Technologies, Vol.4, No.5 (1999) etc.

1 EXECUTIVE SUMMARY

This report summarizes research work carried out in the last three years from 30 May 1999 to 1 June 2002 under the Thailand Research Fund (TRF) contract RTA/04/2442. The purpose of this project is to strengthen the existing Forum for Theoretical Science (FTS) as the Center of Excellence (CE) in Theoretical Sciences by expanding the scope of theoretical science research to cover theoretical biology as well as nanoscience. To achieve this goal it was suggested that a close collaboration between the research institutes as well as universities in Thailand was necessary. The proposal also includes the close collaboration among the ASEAN countries as well as the Universities in the developed world such as USA, France, Germany and Sweden etc. The topics of research should lead to the frontiers of research. Based on this objective it was suggested to carry out 11 topics for research. The outline of the research work on the above topics are submitted to TRF as follows.

1.1 Exciton in Quantum Wells:

The classical treatment of exciton motion in a disordered interface potential is unable to explain the inhomogeneous broadening and consequent asymmetry of exciton lines in two dimensional system. Early attempts to obtain analytical closed-form of the exciton spectra in the presence of disorder within the quantum-mechanical theory were restricted to obtaining the spectral density function in one dimension with a specific type of statistical random potential distribution such as white noise potential. Most of the present theoretical studies are based on the solution of Schrodinger equation of the exciton center of mass motion. In this research we apply the Feynman path integral to study the asymmetric shape, line broadening and low energy shift of the optical absorption spectrum for the two dimensional quantum well [1].

1.2 Optical Absorption of Excitons:

The optical density function of a single quantum well for two-dimensional exciton moving in a random potential in the interfacial plane generated by fluctuations of the quantum well thickness is calculated using the Feynman path integral method. The random potential distribution is assumed to be Gaussion statistics. The calculated optical density function is asymmetrically broadened. The magnitude of the peak is reduced and the maximum is shifted to lower energy as the disorder increases in agreement with other theoretical results as well as experimental time-resolved photoluminescence.

These optical density function properties have technological importance because it has been employed as the active region in the blue-green injector laser diode. The detailed discussion of the Exciton line width was also given in [2]. The results of this research work can be extended to include several quantum wells and then can be applicable to the study of nanotechnology.

1.3 Vortex Dynamics and Magnus Force:

In recent years the interest in vortex motion in superconductivity has revived mainly due to the advent of high temperature superconductivity. As a consequence of the peculiar material properties such as the sign change in the Hall effect, the physics of votices in high temperature superconductivity shows many new aspects not encountered in conventional superconductivity. This Hall anomaly cannot be understood within the framework of the BCS theory. The study of various forces such as the Magnus force acting on the vortex is important for understanding the vortex tunnelling out of the pinning potential. Also the study of vortex dynamics allows us to understand the Magnus force driven motion of vortex in the presence of dissipation. The mathematical derivation of the Magnus force is given in [3]. A more rigorous derivation of Magnus force and the relation of this force to the Hellmann-Feynman force is given in the paper [4]. This rigorous derivation confirms the existence of the Magnus force in the super fluid system. The relationship with the Hellmann-Feynman force may give an insight into other problems in Atomic and Condensed Matter Physics.

1.4 Effective Mass of Vortex :

Recently there has been experimental evidence to show that the initial mass of a moving vortex could affect the dynamics of the vortex. This phenomenon is not fully understood. This is due to the lack of a good understanding of the Magnus force driven vortex in the presence of dissipation. The motion of vortex causes a dipolar density distortion and an associated electric field which is screened. The energy cost of the density distortion as well as the related screened electric field contribute to the vortex mass which is small because of efficient screening. In this research we have succeeded to derive the effective mass of the vortex using the Feynman path integral approach. The result was presented at the [5].

1.5 Vortex Tunneling:

we have studied the influence of pinning, dissipation, and Magnus force on vortex escaping when the potential, which contains both the contribution from Magnus force and pinning potential in y direction, is modeled by the metastable cubic plus quadratic form and the pinning potential in x direction is approximated by the harmonic potential. The equation for determining the crossover temperature is derived. This equation leads us to define the localization criterion of a vortex at finite dissipation and temperature. The criterion shows that, at any temperature and dissipation, a vortex always escapes from the well when the pinning potential in x direction is presented while it is localized in the well for strongly enough Magnus force when the pinning potential in x direction is absent. Moreover, this criterion also leads us to define the effective mass of a vortex in the sense that when a damped vortex decides to escape from the well, it can be effectively viewed as an undamped vortex of a new bigger mass called effective mass. The effective mass is equal to the original mass plus the extra mass originated from the environment and can be viewed as the total mass. This work was presented as the poster session in the RGJ-Ph.D.Congress III meeting held at Jomtian Palm Beach Hotel at Pathaya Cholbury from 25-27 April 2002 and was recognized as the best poster presentation in the physical sciences section [6].

1.6 Dilute Bose Gas in Harmonic Trap:

The recent remarkable experimental demonstration of the Bose-Einstein condensation of dilute ultra cold alkaline atoms in the harmonic trap has stimulated a renewed interest in the ground state energy of the system. Baym and Pethick had shown how to obtain the ground state property using the variation principle. In a series of Master degree theses we have applied the path integral method and show that for the short range interaction with delta interaction potential we obtain the ground state energy which compares well with the variational approach of Baym and Pethick. We have also generalized calculation to include the long range interaction. The ground state energy and the wave function of the condensate are obtained. The calculations are presented in a series of Master theses [7-9]. The response of the noninteracting Boson system under switching of the trap frequency and critical temperature for Boson Pairing in 2D triangular lattice is given in the Ph.D. technical reports [10-11].

1.7 Path integral Treatment of Entangled Polymers:

The theory pertaining to the excluded volume effect in a single polymer chain is one of the central problem in the field of polymer solution theory. The effect of the interaction between the segments which are far apart along a chain is often called the long-range interaction in contrast to the short range interaction representing the interaction among a few neighboring segments. For several polymer chains the problem of entanglement has to be considered. In this research work we consider only single polymer chain with excluded volume. The main result achieved is the calculation of the average mean square displacement at any length of the polymer. The main contribution is that this method allows us to discuss and compare with several models. The method can also be used to discuss the weak interaction and strong interaction in the single formulation. The full detailed calculations are presented and published in the proceedings of the first workshop on "Biological Physics 2000" held at Chulalongkorn University September 18-22, 2000 with the title "Path Integral Approach to a Single Polymer Chain with Excluded Volume Effect" The editors of the proceedings are V. Sa-yakanit. L. Matsson and H. Frauenfelder [10].

1.8 Transport Properties of Metallic Hydrogen:

The first confirmed formation of a metallic state of hydrogen was announced at the March Meeting by scientists at Lawrence Livermore National Laboratory. Metallic hydrogen was achieved in a sample of fluid hydrogen, using a two-stage gas gun to create enormous shock pressure on a target containing liquid hydrogen cooled to 20K.The research direction will be aimed at learning more about the dependence of metallization pressure on temperatures achieved in liquid hydrogen, which is vital for laboratory applications. It was long thought that the road to metallic hydrogen lay with crystalline hydrogen rather than with the disordered fluid phase. According to Neil Ashcroft of Cornell University, dynamic shock techniques to achieve high pressures were first introduced in 1942. Optical evidence of a new phase of hydrogen has been previously reported by scientists at the Carnegie Institute of Washington's Geophysics Laboratory, using an experimental approach that involves crushing microscopic-sized samples of crystalline hydrogen between diamond anvils, achieving pressures up to 2.5 Mbar, but without establishing metallic character. Metallic character is most directly established by electrical conductivity measurements, which are not yet possible in diamond anvil cells at such high pressures.

Ziman had developed a simple multiple scattering theory to explain liquid

metals and alloy. In this research we apply the Ziman theory to liquid metallic Hydrogen. The result of this research work is presented as a master degree thesis [13].

1.9 Magnetic Filtration Nonlinear Effective Dielectric Constant of Composite Materials:

The theory of magnetic filtration has been investigated by several authors especially by Watson. However most of the theories proposed are based on the simplest single collector model. Watson has developed a theory to explain the capture of weakly magnetic particles carried by the fluid of potential flow. The theoretical model used consists of an isolated fine ferromagnetic cylindrical wire in the background of uniform magnetic field. In this research we generalize the theory of Watson which is extended by using the effective medium treatment to predict the magnetic field around the filter matrices consisting of parallel wire distributed randomly. The effective medium treatment is applied to study the conductivity of composite materials which consist of particles disperse randomly in a host medium. The captured radius results of this study are reported and compared with the model of Watson based on single-wire model. Finally the criteria for validity of single-wire model used to determine the magnetic field around the filter matrices are discussed [14].

1.10 Mesoscopic and Low Dimensional Physics:

The problem of a heavily doped semiconductor tends to be like a metal at low bias voltage. If we include the finite-size effect this will bring us to something called the Mesoscopic system. This includes the quantum dot and quantum wire and quasicrystals. In the past decade, rapid progress has been made in Mesoscopic physics. The electronic transport properties of Sierpinski lattices in one-dimension with tight binding model is studied [15]. Since the discovery of the icosahedral quasicrystals in Al-Mn alloys,the quasicrystals with noncrystallographic symmetry, such as decagonal, dodecagonal and octagonal phases have been extensively studied. In this direction we have derived the equation of wave propagating in the cubic quasicrystals and determine the phase velocity of wave propagation which allow us to derive the specific heat of the cubic quasicrystals. This research work is published in [16].

1.11 Mathematical Activities:

The diamond operator and the ultra-hyperbolic operator has been introduced by Kanathai. The purpose of his research is to study the properties of these operators such as the boundness property, Fourier transform and also the Fourier transform of their convolutions. Given these properties the partial differential equation and convolution equation are studied in details .It is found that the convolution equation is related to ultra-hyperbolic equation and is found also that the solution of convolution equation is the singular distribution. At present the main directions of research are Sequence Spaces and combinatorics. Under the strong leadership of Prof.A.Kanathai from Chieng Mai University an Analysis Research group has been established and a series of papers related to the Diamond operator and ultra-hyperbolic operator have been published in several journals [17-20].

1.12 International Materials Research Centers

The National Science Foundation (NSF) of the USA is proposing the support a few world wide "International Materials Reseach Centers". This international centers would consist of a well established Materials Research Labaratory in the USA, which is already one of the NSF national centers, plus some selected Research Centers outside the USA especially in emerging nations. The goal is to bring these centers together into a global network and conduct collaborative research, exchange scientists, hold workshops and train young scientists. The Laboratory for Research on the Structure of Matter at the University of Pennsylvania has submitted a proposal to the NSF to create one of these International Materials Research centers (IMRC). The forum for Theoretical Science as well as the ICTP in Trieste has been selected to be two of the participating Research centers of this global IMRC. This IMRC will focus on biological materials. It will greatly assist FTS in developing productive collaborations with leading centers in this field in the world. It will open opportunities for young Thai scientists to participate in cutting edge research and to work with the best scientists in the world.

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2 CONTENTS OF THE RESEARCH PROGRAMS

2.1 INTRODUCTION

2.1.1 Feynman path integrals

In classical deterministic physics, time evolution of dynamical systems is governed by the least action principle. The Newton classical equations of motion or the law of acceleration can be written as

$$mx''(\tau) = F \tag{1}$$

where $x''(\tau)$ and F denote the second derivative and the external force respectively. This equation can be viewed as the Euler-Lagrange equation

$$\frac{d}{d\tau}\left(\frac{\partial L(x'(\tau), x(\tau), \tau)}{\partial x'(\tau)} - \frac{\partial L(x'(\tau), x(\tau), \tau)}{\partial x(\tau)}\right) = 0 \tag{2}$$

where L is the Lagrangian of the system and $x'(\tau)$denoted as the first derivative of $x(\tau)$. The action functional Srepresenting the dynamical system,is defined as the time integral of the Lagrangian function L

$$S(x'(t), x(0), t) = \int_0^t d\tau L(x'(\tau), x(\tau), \tau) \tag{3}$$

Their trajectories solutions representing the classical dynamical system obtained by minimizing the action functional or the least action principle [1]

$$\delta \;\; S(x'(t), x(0), t) = 0. \tag{4}$$

In quantum physics, one talks about probabilities of different paths quantum (stochastic) dynamical system . According to Feynman, one defines a measure on the set of all possible paths from the initial state $x(0)$ to the final state $x(t)$ of the quantum dynamical system,and expectation values of various quantities dependent upon the paths are given by a path integral or sum over all possible paths from time 0 to time t. The action functional assigns a real number to each path and the exponential of minus this number gives weight of the path in the path integral representation. This formula constitutes a basis for practical calculations of the path-dependent propagator.

$$P\left(x(t), x(0), t\right) = \int_{x(0)}^{x(t)} D(x(\tau)) \exp\left(-\frac{i}{\hbar}\int_0^t d\tau L(x'(\tau), x(\tau), \tau)\right) \tag{5}$$

where $\hbar$ is the plank constant. Path integrals are a basic tool of modern quantum physics. They were introduced by Richard Feynman in 1948 [2,3]. This path integral representation of the propagator can also be derived from the partial differential equation describing Schrodinger equation in quantum mechanics

$$-\frac{i}{\hbar}\frac{\partial\Psi(x,t)}{\partial t} = H(x,t)\,\Psi(x,t) \tag{6}$$

where H denotes the Hamiltonian of the system and is related to the Lagrangian as

$$H(x,t) = p(t)\,x(t) - L(x,t) \tag{7}$$

The wave function $\Psi(x,t)$ representing the probability amplitude is related to the propagator through the spectral resolution

$$P\left(x(t), x(0), t\right) = \sum \overset{*}{\Psi}_n(x,t)\,\Psi_n(x,t)\exp\left(-\frac{i}{\hbar}E_n\right) \tag{8}$$

where E_n is the eigen energy of the schrodinger equation. Finally for $\hbar \to 0$ the classical path is dominated and the path integral representation is reduced to the Euler-Lagrange equations.

2.1.2 Methods and problems

In this report we apply the Feynman Path Integral method to condensed matter physics as well as Biological Physics and Econophysics. The method is based on the Lagrangian approach to principle of least action and demonstrated that Feynman path integrals constitute both a natural theoretical concept and a practical computational tool. We first introduce the effective model action arising from a particle or a system of particles coupled to the environment or reservoir. This environment is in general comprised of many degrees of freedom. photons, phonons, plasmons etc. After eliminating the environmental degree of freedom one obtains the effective model action. In general these effective model actions are non-local in time and therefore the path integrals associated with these model actions cannot be evaluated in closed form.

These problems can be solved by following the method developed by Feynman in handling the polaron problem .The main idea is to introduce the non local quadratic action to simulated general effective non-local action arising from the system coupling to reservoir. The method developed by Feynman for handling the polarons had been extended by Sa-yakanit in handling the disordered systems and several problems in condensed matter physics.

2.2 MODEL SYSTEM

2.2.1 Effective Model Action

Consider a system with one or a few degrees of freedom which is coupled to huge environment and imagine that the environment is represented by a heat bath or reservoir. The interaction of the system with each individual degree of freedom is proportional to the inverse of the volume of the reservoir. Hence the coupling to an individual bath mode is weak. Therefore it is physically reasonable to assume that the system-reservoir coupling is linear. This property allows us to eliminate the environment exactly. The most general form of the action for the global system S is

$$S = S_p + S_I + S_r \tag{9}$$

where S_p, S_I and S_r are actions of particle ,interaction and environment or reservoir respectively. After eliminating the environmental degree of freedom one ends up with the following effective action S

$$S\left(x'\left(t\right), x\left(0\right), t\right) = \int_0^t \frac{m}{2} x'^2 d\tau + \int_0^t \int_0^t d\tau d\sigma W\left[x\left(\tau\right) - x\left(\sigma\right)\right] \tag{10}$$

where $W\left[x\left(\tau\right) - x\left(\sigma\right)\right]$ denotes the non local correlation function arising from eliminating the environmental degree of freedom. Following Feynman the propagator $P\left(x\left(t\right), x\left(0\right), t\right)$ associated with the effective action can be written as

$$\begin{aligned} P\left(x\left(t\right), x\left(0\right), t\right) &= \int_{x(0)}^{x(t)} D\left(x\left(\tau\right)\right) \\ &\exp\left(-\frac{i}{h}\int_0^t \frac{m}{2} x'^2 d\tau + \int_0^t \int_0^t d\tau d\sigma W\left[x\left(\tau\right) - x\left(\sigma\right)\right]\right) \end{aligned} \tag{11}$$

where the integral notation represents the sum over all paths$x\left(\tau\right)$ connecting the initial and final space-time points $x\left(0\right)$, and $x\left(t\right)$ respectively. For each path there is a weighting factor given by $\exp\left(-\frac{i}{h} S\left(x'\left(t\right), x\left(0\right), t\right)\right)$.

In what follows we shall present examples how the effective actions arise by eliminating the environmental degree of freedom.

2.3 Polarons

A polaron is an electron moving in a polar crystal together with the self induced polarization of the lattice. This self induced polarization is a consequence of the electron -phonon interaction. The polaron tends to have a

lower energy and higher effective mass compared to that of a bare electron. Since the action being quadratic in the phonon coordinates, the path integral over this coordinates can be performed exactly. Once the phonon coordinate being eliminated, the problem is reduced to the path integrals of a nonlocal effective action [5].

$$S\left(x'\left(t\right),x\left(0\right),t\right)=\int_0^t\frac{m}{2}x'^2d\tau+\alpha\int_0^t\int_0^t d\tau d\sigma\frac{\exp-\omega\left|\tau-\sigma\right|}{\left|x\left(\tau\right)-x\left(\sigma\right)\right|} \tag{12}$$

where α and ω denote the strength of the interaction and frequency of the optical phonon respectively. This action was first discussed by Feynman to obtain the ground state energy and effective mass of the polaron. The ground state energy and effective mass of the polaron had also been applied and extended by Sa-yakanit [6,7].

2.4 Fluctuons

The fluctuon concept is close to that of the polaron and in some degree can be considered as a generalization of the polaron problem. Special electronic states resemble the polaron-type self-localized state but different from polaron are that the fluctuon is formed in the disordered environment with fluctuation of the concentration such as amorphous materials, heavily doped semiconductors. One can model this problem as an electron motion in the random potential. The random potential can be taken as Poisson or Gaussion distribution. Upon eliminating the random potential one obtains the quasi particle call Fluctuon. For the case of heavily doped semiconductors effective model action takes the form

$$S\left(x'\left(t\right),x\left(0\right),t\right)=\int_0^t\frac{m}{2}x'^2d\tau+\int_0^t\int_0^t dtds\xi_Q exp(-Q(x(t)-x(s)) \tag{13}$$

with ξ_Q = fluctuation parameter having the dimension of energy squared and Q denotes the inverse screening correlation length of the system. This problem had been applied to heavily doped semiconductors[8-12] and Urbach tails [13] in amorphous materials, semiconductors.

2.5 Plasmarons

The electron-plasmon coupling in solids has been discussed by many authors using various methods such as the perturbation method and the dielectic formulation. The interaction of individual electron with plasmon can be described in terms of the Frolich-type interaction in analogy with the polaron

problem. Upon eliminating the plasmon degree of freedom one obtains the effective action. The quasi particle of this problem is called Plasmaron.

$$\begin{aligned} S\left(x'\left(t\right),x\left(0\right),t\right) &= \int_0^t \frac{m}{2}x'^2 d\tau \\ &+ \int_0^t \int_0^t d\tau d\sigma \int_0^\infty \frac{dk}{\omega\left(k\right)} \frac{\cos\left(\omega_p\left(k\right)t/2 - \left|\tau-\sigma\right|\right)}{\sin\left(\omega_p\left(k\right)t/2\right)} \\ &\times \exp\left(ik.\left(x\left(\tau\right)-x\left(\sigma\right)\right)\right) \end{aligned} \tag{14}$$

where $\omega p\left(k\right)$ is the k-dependent plasmon frequency and is given by

$$\omega_p\left(k\right) = \omega_p^o + \alpha k^2 + \beta k^4 \tag{15}$$

where ω_p^o is the plasma frequency, α and β are two numerical constants determined by satisfying the sum rules.

The ground state energy and the effective mass of the Plasmaron are calculated and used to discuss the Wigner crystallizations. The detailed calculation is discussed and given in [14,15].

2.6 Magnus force

The argument for the existing of a Magnus force was discussed by several authors[16]. It was found that the existence of the Magnus force is a general property of the vortex line arising from the influence of the presence of disordered environment. Since then there have been several attempts to derive the Magnus force from different fundamental approaches such as by Chern-SimomTheory and Feynman-Hellmann Theorem. The problem arises from the vortex coupled to the heat bath which contains an infinite set of oscillators. After eliminating the environmental degree of freedom one obtains the following non local action effective action

$$\begin{aligned} S\left(x'\left(t\right),x\left(0\right),t\right) &= \int_0^t \frac{m}{2}x'^2 d\tau + \int_0^t \int_0^\tau d\tau d\sigma \\ &\times \frac{M\omega^2\Omega_x}{8\sin\left(\Omega_x t\right)} \left[\cos\left(\Omega_x\left(t-\tau\right)\right)\cos\left(\Omega_x\sigma\right)\right] \end{aligned} \tag{16}$$

This effective action had been used to discuss several problems such as the vortex tunnelling out of the pinning potential containing the Magnus force and Lorenz force of the high T_c superconductivity. The derivation of Magnus force from the first principle and the relationship to the Feynman-Hellmann force as well as to the Lorenz force are given in [16,17].

2.7 Polymers

A polymer consists of essentially a large number of repeated molecular chains called monomers. These chains can be simple as for example in polyethylene or can be very complex as in DNA. Edwards [18] was the first to apply the path integral techniques to study the polymer chain problems and obtained the configurational probabilities of molecular chains in thermodynamic equilibrium. The chain model of polymers has been used for simulating configuration behavior of polymers with short range and long range interaction between segments along the chain of length L. The effective action in this case can be written as for the case of excluded volume problem

$$S\left(x'\left(t\right),x\left(0\right),t\right)=\int_{0}^{L}\frac{m}{2}x'^{2}d\tau+\int_{0}^{L}\int_{0}^{L}d\tau d\sigma\xi_{l}\delta\left(x\left(\tau\right)-x\left(\sigma\right)\right) \quad (17)$$

where $W\left[x\left(\tau\right)-x\left(\sigma\right)\right]$=$\xi\delta\left(x\left(\tau\right)-x\left(\sigma\right)\right)$ is the correlation function with ξ as the amplitude of fluctuation. This action is identical with the white noise problem in disordered system. The main problem is to calculate the mean square distance $\left\langle R^{2}\right\rangle$ which can be used to obtain other physical properties of the polymers. A comparison with the approach developed by Edwards is given [18].

2.8 Quantum Well

An electron confined to the narrow potential well in the interface of the $GaAs/Al_xGa_{1-x}As$ heterostructure forms a quasi-two dimensional electron gas. Quantizations of the electronic motion perpendicular to the interface leads to a series of quantized energy levels of the potential well. The charged donors are distributed in the highly doped region with the spacer layer thickness d. The effective action is

$$\begin{aligned}S\left(x'\left(t\right),x\left(0\right),t\right) &= \int_{0}^{t}\frac{m}{2}x'^{2}d\tau+\int_{0}^{t}\int_{0}^{t}d\tau d\sigma\int_{0}^{\infty}dqn_{I}\\ &\times\left(\frac{Zr^{2}}{8\epsilon_{0}\epsilon_{s}a}\right)\frac{e^{-2qs}}{2q}\frac{\left(1-ed\right)}{q^{4}\epsilon\left(q\right)^{2}}\exp\left(iq(x\left(\tau\right)-x\left(\sigma\right)\right)\end{aligned} \quad (18)$$

where $\epsilon\left(q\right)$ is the dielectric constant in the Thomas Fermi approximation. This correlation is used to obtain the density of states of the quantum Well [19,20,21].

2.9 Quantum Hall

Two dimensional electron system in a perpendicular magnetic field displays fascinating quantum oscillation. Examples are two dimensional electrons confined to interfaces in GaAs/Al_xGa_{1-x}As layered heterostructure. The correlation in this case is similar to the polymer problem except that in this problem it is a two-dimensional system. The effective action is

$$S\left(x'\left(t\right),x\left(0\right),t\right)=\int_0^t\frac{m}{2}x'^2d\tau+\int_0^t\int_0^t d\tau d\sigma\ \xi_L\exp\left(-\frac{\left(x\left(\tau\right)-x\left(\sigma\right)\right)^2}{L}\right) \tag{19}$$

with ξ_L as the amplitude of fluctuation and L as the correlation length. The density of states as well as the mobility of the Quantum Hall problems are calculated and are given in [22-27].

2.10 Excitons

The bound electron-hole pair is called Exciton. Exciton can be formed in every insulating crystal. All Excitons are unstable with respect to environment and ultimately decay into the recombination process. Exciton can be formed both in three or two dimensions. Currently, Exciton in two dimension is being studied due to its contribution to the understanding of the Quantum well problem. The classical treatment of Exciton motion in disordered interface potential is unable to explain the inhomogeneous broadening of the exciton line in the photo luminescence spectrum due to the sensitivity of the islands. The main interest is to calculate the line width of the exciton due to the interface roughness of the sample and the statistical well-width fluctuation arising from local thickness of the quantum well during the crystal-growth process. The effective action now takes the form of

$$S\left(x'\left(t\right),x\left(0\right),t\right)=\int_0^t\frac{m}{2}x'^2d\tau+\int_0^t\int_0^t d\tau d\sigma\ \xi_l\exp\left(-\frac{\left(x\left(\tau\right)-x\left(\sigma\right)\right)^2}{L}\right) \tag{20}$$

In this case it can be taken the same as the case of Quantum Hall except that this is a two-dimensional system. The effect of the random well width of the exciton and the optical absorption of the exciton are given in [21].

2.11 Biological Physics

In the transport process of a complex system such as molecules in a complex environment the barrier-crossing reaction rate can be treated as classical

chemical kinetics. For example in the case of carbon monoxide recombination with myoglobin the reaction process needs a higher barrier rate equation of a highly non exponential property. The simple model of treating this problem is to assume that the fluctuation relaxes exponentially according to the stretched exponential law. The survival probability associated with this reaction process whose environment is described by a generalized Langevin equation can be reformulated in terms of path integral representation. Then this problem is equivalent to considering the reaction coordinate coupled to the environment which in this case is a set of infinite number of oscillators. By eliminating the environmental degree of freedom we obtain the effective action

$$\begin{aligned} S_0\left(x'\left(t\right),x\left(0\right),t\right) &= \int_0^t \frac{m}{2}x'^2 d\tau + \frac{\kappa\omega}{8}\int_0^t\int_0^t d\tau d\sigma J\left(\omega\right) \\ &\times \frac{\cos(\omega t/2-|\tau-\sigma|)}{\sin\left(\omega t/2\right)}\left[x\left(\tau\right)-x\left(\sigma\right)\right]^2 \end{aligned} \tag{21}$$

where κ and ω are two variational parameters. $J\left(\omega\right)$ denotes the spectral function and is given by

$$J\left(\omega\right) = \frac{\pi}{2})\sum m_j\kappa_j\omega_j\delta\left(\omega\_\omega_j\right) \tag{22}$$

with $\omega_j = \sqrt{\frac{\kappa_j}{m_j}}$ and the summation is carried to infinity to represent the heat bath of the system. The detailed calculations of this problem is given in [22].

2.12 Econophysics

The aim of many physicists working in the field of Econophysics is to develop statistical models that predict the probability that the price of stocks or shares will go up or down. Properties like the distribution of extreme events, such as stock market crashes, and scaling behavior have been explored with very large sets of high frequency data. For instance, there are reported results on the behavior of about 40 million equity returns from the New York Stock Exchange. In simple terms, these reports compared how fluctuations in the prices of stocks and shares compared with a Gaussian distribution. The results confirm that financial assets are definitely riskier than the Gaussian random walk behavior would predict. To overcome this problem the path integral formulation is used to handle this stochastic behavior. The use of path integral does not need any reference to the Black-Scholes equation. The most simple example is to apply the path integral to the Vacicek model. The conventional method to handle the Vacicek model is to study the generalized

Langevin equation for the short rate r. The Vacicek model then can be written in terms of path integral. The model can be used to study the bond price as a specific claim. Using the probability density derived from the stochastic equation, one can write down the action associated with the Vacicek model as

$$S = \frac{2}{\sigma^2} \int ds(x'(s) - a(b - x(s)))^2 \tag{23}$$

where σ is the volatility of the short rate and a,b are constants. One can show that for a zero bond with the short rate environment, this equation can be reduced to the Vacicek dynamic equation. The path integral can also be used to conveniently derive other equations such as the Black-Scholes equation.

The path integral approach to financial modeling is known to a number of finance practitioners with prior quantum physics background. Applications of Feynman's path integrals to financial modeling were pioneered in the mid-eighties by Jan Dash [23,24], an elementary particle physicist currently working in financial industry.

3 METHOD OF CALCULATIONS

3.1 Quadratic Model Trial Action

The above few examples give us general ideas how the effective model action can be derived. These systems in general cannot be solved analytically. Therefore some methods of approximation have to be used in order to carry out the calculation. One can use the perturbation expansions or carrying out the numerical calculation using Monte Carlo method. In this research work we shall follow the variational method developed by Feynman for handling the polaron problem. This method has been proved to be very powerful and allows the calculation to be carrying out analytically. The method is also developed and extended by Sa-yakanit for the condensed matter physics. In order to be able to carry out the calculation analytically, the trial model action has to be introduced,

$$\begin{aligned} S_0\left(x'\left(t\right), x\left(0\right), t : \kappa, \omega\right) &= \int_0^t \frac{m}{2} x'^2 d\tau + \frac{\kappa\omega}{8} \int_0^t \int_0^t d\tau d\sigma \\ &\quad \times \frac{\cos(\omega t/2 - |\tau - \sigma|)}{\sin\left(\omega t/2\right)} \left[x\left(\tau\right) - x\left(\sigma\right)\right]^2 \end{aligned} \tag{24}$$

where κ and ω are two variational parameters to be determined. This model non-local harmonic trial action in principle can be calculated analytically.

The exact solution of this trial action is given in [4]. The physical meaning of this action is that an electron is coupled to the harmonic force with coupling constant κ and fictitious mass m with harmonic frequency $\omega = \sqrt{\frac{\kappa}{m}}$). Once the model trial action is given one can calculate the propagator of the system. According to Feynman the propagator can be written in terms of path integrals

$$P\left(x\left(t\right), x\left(0\right), t\right) = \int_{x(0)}^{x(t)} D\left(x\left(\tau\right)\right) \exp\left(-\frac{i}{h}\int_0^t \frac{m}{2}x'^2 d\tau + \int_0^t \int_0^t d\tau d\sigma W\left[x\left(\tau\right) - x\left(\sigma\right)\right]\right) \tag{25}$$

This propagator in general cannot be performed analytically and therefore one must try to solve this propagator by some approximations. One of the very powerful method developed by Feynman is to use the variational principle. In this method one can rewrite the propagator average with respect to the trial action propagator,

$$P\left(x\left(t\right), x\left(0\right), t\right) = P_0\left(x\left(t\right), x\left(0\right), t\right) \langle \int_{x(0)}^{x(t)} D\left(x\left(\tau\right)\right) \exp\left(-\frac{i}{h}\left(S - S_0\right)\right)\rangle_0 \tag{26}$$

where P_0 is the propagator of the model trial action and is defined as

$$P_0\left(x\left(t\right), x\left(0\right), t\right) = \int_{x(0)}^{x(t)} D\left(x\left(\tau\right)\right) \exp\left(-\frac{i}{h} S_0\left(x'\left(t\right), x\left(0\right), t : \kappa, \omega\right)\right) \tag{27}$$

and the symbol $\langle A\rangle_0$ stands for the average of the functional A with respect to $S_0\left(x'\left(t\right), x\left(0\right), t : \kappa, \omega\right)$ and is defined as

$$\langle A\rangle_0 = \frac{\int_{x(0)}^{x(t)} AD\left(x\left(\tau\right)\right) \exp\left(-\frac{i}{h} S_0\left(x'\left(t\right), x\left(0\right), t : \kappa, \omega\right)\right)}{\int_{x(0)}^{x(t)} D\left(x\left(\tau\right)\right) \exp\left(-\frac{i}{h} S_0\left(x'\left(t\right), x\left(0\right), t : \kappa, \omega\right)\right)} \tag{28}$$

3.2 Variational Calculation

To be able to perform the calculation we expand the propagator in a series of cumulant expansions and keep only the first cumulant. The approximate

propagator $P_1\left(x(t),x(0),t\right)$ now takes the form,

$$P_1\left(x(t),x(0),t\right) = P_0\left(x(t),x(0),t\right)\int_{x(0)}^{x(t)} D(x(\tau))\times \exp\langle\left(-\frac{i}{h}(S-S_0)\right)\rangle_0 \quad (29)$$

The justification of this approximation is based on the Jensen inequality.To be able to apply the Jensen inequality we must replace time t by $-ih\beta$ in the above propagators. Since the averages are performed with respect to the trial quadratic non-local action, therefore all calculations can be performed analytically. We may immediately obtain the statistical density matrix by

$$P_1\left(x(\beta),x(0),\beta\right) = P_0\left(x(\beta),x(0),\beta\right) \int_{x(0)}^{x(\beta)} D(x(\tau))\exp\langle-(S-S_0)\rangle_0 \quad (30)$$

Once the propagator is known, the free energy F can be obtained by using the relation

$$F=-\frac{1}{\beta}\ln\int dx(\beta)\,P_1(x(\beta),x(0),\beta)\delta(x(\beta)-x(0)) \quad (31)$$

Furthermore, if the propagator depends only on $x(\beta)-x(0)$ the above equation can be simplified to

$$F=-\frac{1}{\beta}\ln P_1(x(\beta),x(\beta),\beta) \quad (32)$$

The free energy F of the system can now be obtained by using

$$F=F_0+\frac{1}{\beta}\mathrm{diag}\langle-(S(x'(\beta),x(0),\beta)-S_0(x'(\beta),x(0),\beta:\kappa,\omega))\rangle_0 \quad (33)$$

where F_0 is the free energy of the system described by the density matrix associated with S_0 and is given as

$$F_0=-\frac{1}{\beta}\ln P_0(x(\beta),x(\beta),\beta) \quad (34)$$

The ground state energy of the system E obtained by letting $\beta\to\infty$ and we arrive at

$$E(\kappa,\omega) = E_0(\kappa,\omega) + \lim_{\beta\to\infty}\frac{\langle-(S(x'(\beta),x(\beta),\beta)-S_0(x'(\beta),x(\beta),\beta:\kappa,\omega))\rangle_0}{\beta} \quad (35)$$

E_0 being the ground state energy associated with the system characterized by the action functional S_0. Thus we observe that within the first cumulant approximation the task of obtaining the propagator is reduced to evaluating the $P_0\left(x\left(t\right), x\left(0\right), t\right)$ and the $\langle(-\left(S-S_0\right))\rangle_0$.

The results are now containing two variational parameters κ and ω. Carrying out the variational calculation we obtain two sets of coupled equations.

$$\frac{\partial}{\partial\kappa}E\left(\kappa,\omega\right)=0 \tag{36}$$

$$\frac{\partial}{\partial\omega}E\left(\kappa,\omega\right)=0 \tag{37}$$

After solving two sets of coupled equations and substituting back to the approximate propagator we obtain the free energy, the ground state energy,the effective mass as well as wave functions of the system. Thus we have demonstrated that a variety of problems in condensed matter physics can be handled well by using Feynman path integrals method including, Biological Physics as well as Econophysics.

3.3 DISCUSSION

In this report we have demonstrated the powerful method of the Path Integral formulation and have shown that the technique developed by Feynman is very practical for application to a variety of problems[28-36] especially the condensed matter physics . The main idea of this approach is to introduce the non local quadratic action to simulate the general effective non-local action arising from the system coupling to reservoir. In fact the non-local action first appears in Quantum Electrodynamics by Feynman. In that case the reservoir is the photon and upon eliminating the photon degree of freedom one obtains the effective nonlocal action. Feynman used the same idea to handle the polaron problem. The second main idea of this method is that one can modify contribution from each path to be real rather than complex and then employ the variational principle based on the Jensen inequality to determine all thermodynamic and physical properties.

Path integrals are now used to describe stochastic phenomena ranging from Polymer Science [39], Biological Physics [40], modeling of interest rates and the Pricing of Derivative Securities[39-42]. In finance, the fundamental concepts are equilibrium and arbitrage-free pricing. They can be interpreted as finance counterparts of the least action principle. Accordingly, one can consider a Lagrangian function and an action functional for financial models. Since financial models are stochastic, expectation values of various quantities

contingent upon price paths (financial derivatives) are given by Feynman's path integrals, where the action functional for the underlying (risk neutralized) price process defines a measure on the set of all paths. The averages satisfy the Black-Scholes equation [43,44], which is a finance counterpart of the Schrodinger equation.

Finally, it is interesting to mention two recent developments of financial models. The first approach is given in Kleinert in his recent book on the generalization of the option pricing from path integral for non-Gaussion fluctuation [47]. The stochastic calculus and the option price formulas developed in this book will be useful for estimating financial risks of a variety of investments. In particular, it will help develop a more realistic theory for fair option prices. The second development is to employ the Fractional Brownian Motion as a model in finance. One can define the stock price model as Fractional Brownian semi linear stochastic differential equation. This approach was considered by Krvavy from Ukraine [48] and Sottnen and Valkeila [49]. These two authors discussed the fractional Black-Scholes equation on how to define the stochastic integrate, European options in fractional model. It is suggested that FTS should take this opportunity to explore this very exciting field by using path integral in financial market.

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3. Research Teams

รายชื่อกลุ่มวิจัย

ชื่อ-นามสกุล	เมื่อเข้าร่วมโครงการ			ปัจจุบัน		
	ตำแหน่งวิชาการ	สังกัด	ตำแหน่งในโครงการ	ตำแหน่งวิชาการ	สังกัด	สถานภาพปัจจุบัน
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รายชื่อกลุ่มวิจัย

ชื่อ-นามสกุล	เมื่อเข้าร่วมโครงการ			ปัจจุบัน		
	ตำแหน่งวิชาการ	สังกัด	ตำแหน่งในโครงการ	ตำแหน่งวิชาการ	สังกัด	สถานภาพปัจจุบัน
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ชื่อ-นามสกุล	เมื่อเข้าร่วมโครงการ			ปัจจุบัน		
	ตำแหน่งวิชาการ	สังกัด	ตำแหน่งในโครงการ	ตำแหน่งวิชาการ	สังกัด	สถานภาพปัจจุบัน
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ชื่อ-นามสกุล	เมื่อเข้าร่วมโครงการ			ปัจจุบัน		
	ตำแหน่งวิชาการ	สังกัด	ตำแหน่งในโครงการ	ตำแหน่งวิชาการ	สังกัด	สถานภาพปัจจุบัน
18. นายสุชาติ เกศกมลาสน์		ภาควิชาฟิสิกส์ คณะวิทยาศาสตร์ จุฬาลงกรณ์มหาวิทยาลัย	นิสิต ปริญญาโท	อาจารย์	ภาควิชาวิทยาศาสตร์ คณะศิลปะศาสตร์และ วิทยาศาสตร์ มหาวิทยาลัยธุรกิจบัณฑิตย์	ยังอยู่ในโครงการ
19. นายชัชวาล ศรีภักดี		ภาควิชาฟิสิกส์ คณะวิทยาศาสตร์ จุฬาลงกรณ์มหาวิทยาลัย	นิสิต ปริญญาโท	อาจารย์	สถาบันเทคโนโลยีราชมงคล วิทยาเขตพระนครเหนือ	ยังอยู่ในโครงการ
20. นายสรไกร ศรีศุภผล		ภาควิชาฟิสิกส์ คณะวิทยาศาสตร์ จุฬาลงกรณ์มหาวิทยาลัย	นิสิต ปริญญาโท	อาจารย์	ภาควิชาฟิสิกส์ คณะวิทยาศาสตร์ มหาวิทยาลัยบูรพา	ยังอยู่ในโครงการ
21. นายณัฐพล นาคปฐมกุล		ภาควิชาฟิสิกส์ คณะวิทยาศาสตร์ จุฬาลงกรณ์มหาวิทยาลัย	นิสิต ปริญญาโท	อาจารย์	ภาควิชาฟิสิกส์ คณะวิทยาศาสตร์ มหาวิทยาลัยธรรมศาสตร์	ยังอยู่ในโครงการ
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รายชื่อกลุ่มวิจัย

ชื่อ-นามสกุล	เมื่อเข้าร่วมโครงการ			ปัจจุบัน		
	ตำแหน่งวิชาการ	สังกัด	ตำแหน่งในโครงการ	ตำแหน่งวิชาการ	สังกัด	สถานภาพปัจจุบัน
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25. นายอิษฎา ทองกุล		ภาควิชาฟิสิกส์ คณะวิทยาศาสตร์ จุฬาลงกรณ์มหาวิทยาลัย	นิสิตปริญญาตรี		ภาควิชาฟิสิกส์ คณะวิทยาศาสตร์ จุฬาลงกรณ์มหาวิทยาลัย	นิสิตปริญญาโท ยังอยู่ในโครงการ
26. นายพูล ยิ่งประทานพร		ภาควิชาฟิสิกส์ คณะวิทยาศาสตร์ จุฬาลงกรณ์มหาวิทยาลัย	เข้าร่วมภายหลังได้รับทุน		ภาควิชาฟิสิกส์ คณะวิทยาศาสตร์ จุฬาลงกรณ์มหาวิทยาลัย	นิสิตปริญญาโท ยังอยู่ในโครงการ
27. นายโกมินทร์ แก้วผลึก		ภาควิชาฟิสิกส์ คณะวิทยาศาสตร์ จุฬาลงกรณ์มหาวิทยาลัย	เข้าร่วมภายหลังได้รับทุน		ภาควิชาฟิสิกส์ คณะวิทยาศาสตร์ จุฬาลงกรณ์มหาวิทยาลัย	นิสิตปริญญาโท ยังอยู่ในโครงการ
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รายชื่อกลุ่มวิจัย

ชื่อ-นามสกุล	เมื่อเข้าร่วมโครงการ			ปัจจุบัน		
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31. นางสาวสุภัทรา อดุลรัตนานุวัตร		ภาควิชาฟิสิกส์ คณะวิทยาศาสตร์ จุฬาลงกรณ์มหาวิทยาลัย	เข้าร่วมภายหลังได้รับทุน		ภาควิชาฟิสิกส์ คณะวิทยาศาสตร์ จุฬาลงกรณ์มหาวิทยาลัย	นิสิตปริญญาโท ยังอยู่ในโครงการ
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35. นายชนินทร์ เชื้อรามัญ		ฟอรัมวิทยาศาสตร์ทฤษฎี	ผู้ช่วยนักวิจัย		ฟอรัมวิทยาศาสตร์ทฤษฎี	ยังอยู่ในโครงการ
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รายชื่อกลุ่มวิจัย

ชื่อ-นามสกุล	เมื่อเข้าร่วมโครงการ			ปัจจุบัน		
	ตำแหน่งวิชาการ	สังกัด	ตำแหน่งในโครงการ	ตำแหน่งวิชาการ	สังกัด	สถานภาพปัจจุบัน
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4. Output

[1] Sa-yakanit. V., Ph. Roussignol and Slavcheva G. Effect of Random Well-width Fluctuations on the Exciton Optical Absorption Spectrum in Single Quantum Wells, Proceedings of the First NRCT-KOSEF Joint Seminar on Semiconductors, 30 November - 1 December 1999, Bangkok, Thailand (1999).: Impact Factor=0

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Appendix

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Effect of Random Well-width Fluctuations on the Exciton Optical Absorption Spectrum in Single Quantum Wells

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Abstract

The optical density function is calculated in a single quantum well (QW) for 2D-excitons moving in a random potential in the interfacial plane generated by the fluctuations of the quantum well thickness. Assuming Gaussian statistics for the random potential distribution, we have applied the path-integral approach and obtained in the adiabatic approximation two asymptotic analytical expressions for the low- and high-energy tails of the optical absorption spectrum, respectively. In order to obtain the spectrum across the whole energy range an analytical interpolation formula is found between the asymptotic expressions in both cases. The calculated optical density function is asymmetrically broadened, the magnitude of the peak is reduced and the maximum is low-energy-shifted in both cases considered, as the disorder increases, in agreement with other theoretical results. Using the fitting parameters to the time-resolved photoluminescence data of [R. Zimmermann, Il Nuovo Cimento D 17, 1801 (1995)] we find that the path-integral method leads to results for the spectral widths (FWHM) which are closer to those experimentally observable, as compared with results inferred from the perturbation theory approach.

1. General Introduction

The effect of the in-plane interface disorder on the optical properties of the 2D excitons is currently pursued with renewed interest due to its persistence both in cw and time-resolved experiments. In narrow QWs the interfacial disorder generates potential fluctuations resulting in band tails in the exciton density of states composed from localised states. Due to the static disorder the optical response of the Wannier excitons in QW exhibits significant broadening and distinct asymmetry of the exciton line manifested by mixed Lorentz-Gaussian lineshapes [1]. On the other hand, a modification of the exciton radiative lifetime and respectively of the photoluminescence spectra is predicted as a consequence of the presence of interfacial disorder and exciton localisation [2,3]. Besides the influence on the lineshape, substantial Stokes shift between the exciton lines in absorption and photoluminescence spectra is observed at low temperatures [4] due to interface roughness. These phenomena can be viewed as effects of dephasing, or partial breakdown of temporal coherence [5].

In this paper we aim to develop a semi-analytical quantum-mechanical description of the asymmetric exciton line shapes, line broadening and low-energy shift of the optical absorption spectrum for the 2D-excitons in a QW taking into account the exciton localisation in the random potential fluctuations at the interface. The latter is achieved applying Feynman path-integral method for calculation of the band-tail and semiclassical exciton density of states. Our approach will follow mainly [2] where two asymptotic expressions for the optical density function for high- and low-energy tail of the absorption spectrum have been obtained. The high-energy tail of the spectrum calculated in [2], has been obtained using perturbation theory and the low-energy tail is found by the optimal fluctuation technique [11,12] assuming a white-Gaussian-noise correlation function.

In what follows, we shall show that such a semi-analytical approach turns out to be more advantageous compared to the pure numerical computations in 2D [10] and implies linewidths closer to those experimentally observed. In distinction to the method of Efros *et al.* [2], we calculate the optical density function using the general path-integral exciton density of states, derived in [13] assuming Gaussian random potential distribution and a Gaussian binary correlation function. Finally a full 2D exciton absorption spectrum calculation is performed.

2. Theoretical Model and Analytical Calculations

2.1 Optical density function

We shall consider the motion of the 2D exciton in the random potential whose wave function according to [14] can be represented by the following product:

$$\Psi(r_e, r_h) = \Psi(R)\varphi(\rho)\chi_e(z_e)\chi_h(z_h) \qquad (1)$$

where $\mathbf{r}_{e,h}(\rho_{e,h}, z_{e,h})$ are the electron and hole coordinates, respectively in-plane and perpendicular to the plane of a quantum well, $\rho = \rho_e - \rho_h$ is the coordinate of the relative motion of the two carriers, $\mathbf{R} = (m_e\rho_e + m_{hh}\rho_h)/M$ is the exciton's c.o.m. coordinate, $M = m_e + m_{h//}$ is the total heavy-hole exciton mass, m_e, $m_{h//}$, being the electron and heavy hole mass parallel to the interface, $\Psi(\mathbf{R})$ is the exciton's c.o.m. wave function describing its motion in the quantum well plane, $\chi_e(z_e)$ and $\chi_h(z_h)$ are the wave functions for electron and hole motion in z-direction (perpendicular to the interfacial plane) which for the electrons (or the holes) only is that of a particle in a one-dimensional quantum well. $\varphi(\rho)$ is the exciton wave function describing the in-plane relative motion of the electron and the hole.

Within the adiabatic approximation we shall assume that the exciton line is slightly broadened. Therefore the solution for the exciton wave function could be factorized out and thus we end up with a Schrödinger equation for a particle of a mass M in a random adiabatic potential:

$$\left[-\frac{\hbar^2\nabla^2}{2M} + V(\mathbf{R})\right]\psi(\mathbf{R}) = E\psi(\mathbf{R}). \qquad (2)$$

Our model is aiming to find the spectral function of a single particle (exciton center-of-mass)in the field of N scatterers confined in an area S at the interface during its motion near the disordered interface of the quantum well obeying the Hamiltonian:

$$\hat{H} = \hat{H}_0 + V(\mathbf{R}) \qquad (3)$$

where $\hat{H}_0$ is the unperturbed Hamiltonian of the ordered system without randomness and the random in-plane potential $V(\mathbf{R}) = \sum_i v(\mathbf{R} - \mathbf{R}_{0i})$ (Fig. 1) is a superposition of individual scattering potentials $v(\mathbf{R} - \mathbf{R}_{0i})$ representing the 2D random potential generated at a point $\mathbf{R}(x, y)$ in the heterojunction interfacial plane by the local well-width fluctuation located at $\mathbf{R}_{0i}(x_{oi}, y_{oi})$ in the plane.

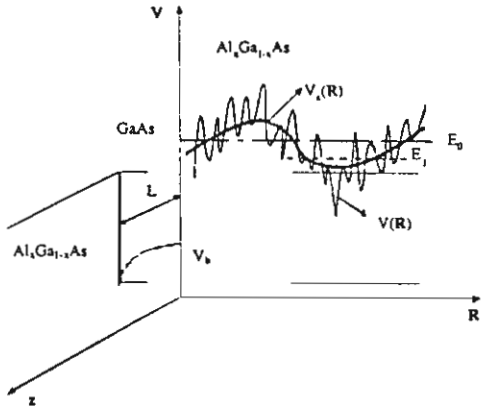

Fig 1. Plot of the random potential V(R) seen by the exciton c.o.m. in the interfacial plane of a single quantum well. Vs(R) is the smoothed potential over the characteristic size of the exiton c.o.m. envelope wave function: $V_s(\mathbf{R}) = \int d^2\mathbf{R}'\Psi^*(\mathbf{R}')V(\mathbf{R}')\Psi(\mathbf{R}')$. E_o is the average potential energy, E_j is the energy of the exciton c.o.m. localised state. L is the width and V_b is the quantum well depth.

The statistical properties of the random potential energy distribution are characterized by its moments. We shall assume a Gaussian statistical distribution which is completely described by its first and second moments, i.e. by the mean potential energy and the binary correlation function:

$$E_0 = \langle V(\mathbf{R})\rangle = \overline{N}_{2D}\int d\mathbf{R}_0 v(\mathbf{R} - \mathbf{R}_0) \qquad (4)$$

$$W(\mathbf{R} - \mathbf{R}') = \langle V(\mathbf{R})V(\mathbf{R}')\rangle = \overline{N}_{2D}\int d\mathbf{R}_0 v(\mathbf{R} - \mathbf{R}_0)v(\mathbf{R}' - \mathbf{R}_0) = \xi_L e^{-|\mathbf{R}-\mathbf{R}'|^2/L^2} \qquad (5)$$

where $\overline{N}_{2D} = N/S$ is the surface density of the scattering centers, L is the correlation length of the random potential fluctuations and ξ_L is the dispersion of the random Gaussian potential which has the dimension of energy squared and in the 2D case is given by:

$$\xi_L = \overline{N}_{2D}\left(\frac{\pi L^2}{4}\right)v_0^2. \qquad (6)$$

In the above expression we have introduced the strength (or amplitude) v_0 of the individual potential according to:

$$v(\mathbf{R} - \mathbf{R}_0) = v_0 e^{-|\mathbf{R}-\mathbf{R}_0|^2/l^2} \qquad (7)$$

and $L = l\sqrt{2}$.

The spectral density function for a 2D Schrödinger particle in a random potential is defined according to [9], by:

$$A(\mathbf{K}_{//}, E) = \frac{1}{S}\left\langle \sum_i \left| \int e^{i\mathbf{K}_{//}\cdot\mathbf{R}}\Psi_i(\mathbf{R})d^2\mathbf{R}\right|^2 \delta(E - E_i)\right\rangle \qquad (8)$$

where $\Psi_i(\mathbf{R})$ is the exciton's center-of-masswave function of the i^{th} exciton state with a corresponding energy E_i, $\mathbf{K}_{//}$ is the 2D-exciton wave vector in the plane parallel to the interface, S- is the normalization area. The above averaging is

performed over all possible configurations of the random potential fluctuations ($\langle ... \rangle$ indicating an average over the statistical ensemble).

Since we shall be interested in the optical absorption spectrum, we wish to calculate the optical density function which represents the inverse Fourier transform of the spectral density Eq.(8):

$$A(E) = \frac{1}{S}\left\langle \sum_i \left| \int d^2\mathbf{R}\Psi_i(\mathbf{R}) \right|^2 \delta(E - E_i) \right\rangle \qquad (9)$$

Then the absorption coefficient can be written as:

$$\alpha(\omega) = \alpha_0 A(E) \qquad (10)$$

where α_0 is a slowly varying function of the excitation frequency ω (see e.g. [15]).

2.2 Path-integral approach for calculation of the optical density function

In order to calculate the optical density function we need to obtain the 2D excitonic DOS. Reformulating the problem in path-integral (PI) terms we need to calculate the average (over all random potential configurations) exciton one-particlepropagator:

$$\overline{G}(\mathbf{R}_2, \mathbf{R}_1; t) = \int D[\mathbf{R}(\tau)] e^{\frac{i}{\hbar}S} \qquad (11)$$

with the boundary conditions: $\mathbf{R}(0) = \mathbf{R}_1$, $\mathbf{R}(t) = \mathbf{R}_2$ and S is the action of the random system, given up to the second-order moment of the random potential distribution by:

$$S = \int_0^t d\tau \left[\frac{M}{2}\dot{\mathbf{R}}^2(\tau) - E_0 + \frac{i}{2\hbar}\int_0^t d\sigma W[\mathbf{R}(\tau) - \mathbf{R}(\sigma)] \right] \qquad (12)$$

whose diagonal elements give the density of states.

$$\rho(E) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{\frac{i}{\hbar}Et}\overline{G}(0,0;t) \qquad (13)$$

The DOS per unit volume in the first cumulant approximation for a Gaussian random potential, with a Gaussian binary correlation function is derived in [13] for the general case of a d-dimensional system:

$$\rho_1(E) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt \left(\frac{M}{2\pi i\hbar t}\right)^{d/2} \left(\frac{\Omega t}{2\sin\frac{\Omega t}{2}}\right)^d exp\left[\frac{d}{2}\left(\frac{\Omega t}{2}ctg\frac{\Omega t}{2} - 1\right) - \frac{1}{2\hbar^2}\xi_L t\int_0^t dx j(x,\Omega)^{-d/2} + \frac{i}{\hbar}(E - E_0)t\right] \qquad (14)$$

where Ω is the non-local harmonic oscillator frequency which is a variational parameter to be determined and the function $j(x,\Omega)$ is given by::

$$j(x,\Omega) = \left(1 + \frac{i\hbar}{M\Omega}\frac{4}{L^2}\frac{\sin\frac{\Omega x}{2}\sin\frac{[\Omega(t-x)]}{2}}{\sin\frac{\Omega t}{2}}\right) = \left(1 + 8i\frac{E_L}{E_\Omega}\frac{\sin\frac{\Omega x}{2}\sin\frac{[\Omega(t-x)]}{2}}{\sin\frac{\Omega t}{2}}\right) \qquad (15)$$

with $E_\Omega = \hbar\Omega$ and $E_L = \frac{\hbar^2}{2ML^2}$ (16)

is the correlation energy (the kinetic energy of localisation over a distance L - the screening length of the random potential fluctuations) representing a measure of the exciton confinement.

Two analytical asymtotic expressions for the 2D exciton DOS (d=2) can be obtained from the above general expression in the so called low-energy limit, i.e. deep in the excitonic band-tail and in the opposite extreme of high-energy, i.e. near to the band edge.

2.2.1 Low-energy limit

We shall be interested in calculating the optical density function in the low-energy tail i.e. the region of negative energies below the unperturbed band edge.

Let us consider first the DOS caclulation in the excitonic band tail. In order to evaluate the ground-state energy contribution to the DOS we have to take the limit $t \to \infty$ of the general DOS expression (14). The 2D exciton DOS deep in the band tail is obtained from that limit, by letting $E \to -\infty$ and minimizing the DOS exponent with respect to the variational parameter $z = \frac{E_\Omega}{E_L}$. Introducing dimensionless normalized energy:

$$v = \frac{E_0 - E}{E_L} \qquad (17)$$

we obtain for the 2D DOS deep in the excitonic band-tail:

$$\rho_T(v) = \left[\frac{1}{E_L L^2}\frac{1}{\xi'^{3/2}}\right] a(v) e^{-\frac{h(v)}{2\xi'}} \qquad (18)$$

with pre-exponential and exponential factors given by:

$$a(v) = \frac{\left(\sqrt{1+4v} - 1\right)^{3/2}\left(\sqrt{1+4v} + 3\right)^{5/2}}{2^{9/2}\pi^{3/2}} \qquad (19)$$

$$b(v)=\frac{1}{2^4}\left(\sqrt{1+4v}-1\right)\left(\sqrt{1+4v}+3\right)^3. \qquad (20)$$

where we have introduced a dimensionless quantity:

$$\xi'=\frac{\xi_L}{E_L^2} \qquad (21)$$

In order to calculate the optical density function, we rewrite (9) in the form of a functional integral over all possible potential fluctuations:

$$A(E)=\frac{1}{S}\int DV.W(V)\sum_i\left|\int d^2\mathbf{R}\Psi_i(\mathbf{R})\right|^2\delta(E-E_i) \qquad (22)$$

where $W(V)$ is the probability of the random potential distribution. Since in the low-energy range we shall be interested only in the ground-state contribution to the density of states (since we have taken the limit $t\to\infty$ in obtaining it), we can consider that the main contribution to the above integral comes from the ground state exciton center-of-masswave function in a harmonic potential well, i.e.

$$\Psi_o(R)=\left(\frac{2\gamma}{\pi}\right)^{1/2}e^{-\gamma R^2} \qquad (23)$$

where

$$\gamma=\frac{M\Omega}{\hbar}=\frac{z}{2L^2} \qquad (24)$$

and z is a variational parameter, the same as that appearing in the band-tail DOS.

Therefore we can take the factor $\left|\int d^2R\Psi_o(R)\right|^2$ out of the functional integral. The remaining functional integral is, by definition, the band-tail density of states $\rho_T(v)$. Substituting γ and z from Eq. (29) and Eq. (22) we obtain the following expression for the low-energy tail of the optical density function:

$$A(v)=\frac{4\pi L^2}{\left(\sqrt{1+4v}-1\right)}\rho_T(v) \qquad (25)$$

2.2.2 High-energy limit

Let us consider now the calculation of the high-energy tail of the optical density function. In order to obtain the high-energy semiclassical Kane limit of the general PI expression for the 2D exciton DOS near to the band edge it is necessary to take the limit $t\to 0$ of Eq. (14) which corresponds to retaining only high-energy excitonic states in the DOS. Introducing dimensionless variables ξ', v we get:

$$\rho_K(v)=\frac{1}{2^{5/2}\pi^{3/2}E_LL^2}e^{-\frac{v^2}{4\xi'}}D_{-1}\left(\frac{v}{\sqrt{\xi'}}\right) \qquad (26)$$

where D_{-1} is the parabolic cylinder function of order -1.

In the opposite extreme - at high enough energies the exciton c.o.m. wave functions $\Psi_i(\mathbf{R})$ are close to plane waves. According to [16] the exciton states close to the delocalized states can be described quite satisfactorily by choosing the c.o.m. envelope wave function of the form:

$$\Psi_i(\mathbf{R})=\frac{A_o}{\sqrt{S}}e^{i\mathbf{K}_i.\mathbf{R}-\gamma R^2},A_o=\left(\frac{2\gamma S}{\pi}\right)^{1/2}. \qquad (27)$$

We shall consider that the main contribution to the configurational average in Eq. (9) at high energies is given by states with an equal shape of the envelope wave function.

Therefore, similarly to the first case (deep in the band tail) we can take the matrix element out of the ensemble averaging and the remaining average gives the semiclassical Kane 2D-exciton DOS Eq. (27).

After directly calculating the matrix element we obtain the following general expression for the optical density function at high-energies:

$$A(v)=\frac{1}{2^{3/2}\sqrt{\pi}}\frac{1}{\gamma L^2E_L}e^{-v^2\left[\frac{1}{(4\gamma L^2)^2}+\frac{1}{4\xi'}\right]}D_{-1}\left(\frac{v}{\sqrt{\xi'}}\right) \qquad (28)$$

from which the following two limiting cases, corresponding to the semiclassical Kane band tail and the free-exciton (continuum states) 2D DOS can be considered:

$$A(v)=\begin{cases}\dfrac{1}{2\sqrt{2\pi}}\dfrac{\sqrt{\xi'}}{\gamma L^2E_L}\dfrac{1}{v}e^{-v^2\left[\frac{1}{(4\gamma L^2)^2}+\frac{1}{2\xi'}\right]}, & \dfrac{v}{\sqrt{\xi'}}>>1\\ \dfrac{1}{2\gamma L^2E_L}\left[1+erf\left(\dfrac{v}{\sqrt{\xi'}}\right)\right]e^{-v^2/(4\gamma L^2)^2}, & \dfrac{v}{\sqrt{\xi'}}<<1\end{cases} \qquad (29)$$

If we take the limit $v\to\infty$ of the free-exciton DOS since for the free excitons the difference between the energy of the exciton c.o.m. and the mean potential energy E_o is expected to be much larger than the localisation energy E_L, we obtain a pure Gaussian exciton lineshape:

$$A(v)=\frac{1}{\gamma L^2E_L}e^{-v^2/(4\gamma L^2)^2}. \qquad (30)$$

The dimensionless parameter $\gamma L^2=z/2$) depends on the variational parameter z introduced in the calculation procedure of the low-energy tail of the spectral density.

2.3 Perturbation theory approach for high-energy tail of the optical density function

Let us calculate the high-energy tail of $A(E)$ using the perturbation theory. In this region the exciton center-of-mass wave functions are close to plane waves.

Using the perturbation theory in the high-energy limit we have:

$$A(E)=\frac{1}{S}\int\frac{d^2K_{\parallel}}{(2\pi)^2}\frac{\left\langle\left|\int V(\mathbf{R})e^{i\mathbf{K}_{\parallel}\cdot\mathbf{R}}d^2\mathbf{R}\right|^2\right\rangle}{E_{K_{\parallel}}^2}\delta\left(E-E_{K_{\parallel}}\right) \tag{31}$$

Let us first calculate the average in the above expression..Substituting the correlation function $\langle V(\mathbf{R})V(\mathbf{R}')\rangle$ from (5) and performing the integration by introducing the new variable $\mathbf{x}=\mathbf{R}-\mathbf{R}'$ (because of the translational invariance in the plane parallel to the interface), we obtain:

$$\left\langle\left|\int V(\mathbf{R})e^{i\mathbf{K}_{\parallel}\cdot\mathbf{R}}d^2\mathbf{R}\right|^2\right\rangle=\xi_L S\pi L^2 e^{-K_{\parallel}^2L^2/4} \tag{31}$$

After performing the integration over 2D in-plane wave vector in (33) and introducing dimensionless parameters, we obtain the following expression:

$$A(v)=\frac{\xi'}{4E_L v^2}e^{-v/4} \tag{32}$$

Comparing Eq. (32) with the path-integral expression (30) at high energies, we can conclude that the perturbation theory result for the high-energy shoulder of the spectrum decays faster than the semiclassical limit of the path-integral result, resulting in a broader spectrum.

3. Numerical Computations and Results

In Sec. 2 we have obtained using a path integral method low-energy (given by Eq. (25), and (18), (19), (20)), and high-energy Eq. (28) asymptotic expressions for the optical density function and an alternative high-energy asymptotics resulting from the perturbation theory Eq. (32). Since we are interested in the spectrum across the whole energy range, an interpolation function between Eq. (25) and Eq. (32), hereinafter referred to as case 1, and on the other hand - between Eq. (25) and Eq. (28), referredas case 2, has to be sought. The interpolation function in both cases has been found by performing a nonlinear fitting procedure based on the chi-squared minimization criterion using the proper normalization:

$$A(v,\xi')=\begin{cases}\dfrac{\xi' e^{-1.03975.v/\xi'}\left(0.53665.v^2+1.35851.v+0.81927\right)}{\left(v^2+0.28551\right)^2\left[4.21614.\sqrt{\xi'}+10.01300.e^{0.296863/\xi'}\left(\xi'-0.40664\right).erfc\left(\dfrac{0.54485}{\sqrt{\xi'}}\right)\right]}, & case1\\[2ex] \dfrac{0.23810.e^{-2.83076/\xi'}}{erfc\left(\dfrac{1.68249}{\sqrt{\xi'}}\right)}\dfrac{e^{-1.06150.v^1/\xi'}(v+2.18072)}{v^2+2.66678}, & case2\end{cases} \tag{33}$$

In our calculations we have introduced basically two disorder parameters, namely the variance (dispersion) of the random potential σ (or equivalently ξ_L) and the correlation energy E_L. In order to study the effect of changing the correlation length of the potential fluctuations on the optical absorption spectrum we have fixed the variance at a value of σ=0.5 *meV* varying the correlation energy (or equivalently the correlation length). The interval of variation of the correlation lengths has been chosen in conformity with the value for the correlation energy E_L=0.12 *meV* of Zimmermann [6], which gives L≈9.61 nm., i.e. L varies from 7 nm to 70 nm. The calculated optical density functions are presented in Figures 2 (a, b).

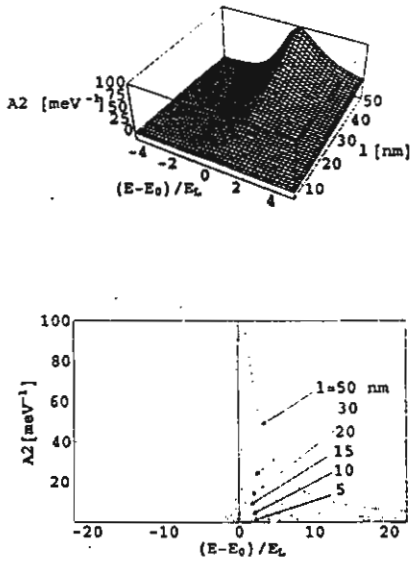

Fig 2. (a) 3D plot of the optical density function corresponding to case 2 vs the energy, normalized with respect to the exciton correlation energy E_L, and the correlation length l.; (b) cross-sections of (a): plots of the optical density function vs normalized energy corresponding to case 2 for l=5, 10, 15, 20, 50 nm.

We have introduced the new variable l, according to: $L = l\sqrt{2}$. It can be seen (Figure 2) that increasing the correlation length (or equivalently l) and approaching the classical limit (i.e. $L \to \infty$ corresponding to perfect interface) the optical absorption spectrum tends to the free-exciton δ-peak. In the opposite limit - decreasing the correlation length continuous broadening of the exciton linewidth is observed, with a decrease in the peak magnitude and low-energy shift of the maximum. In this case we approach the quantum case of strong screening of the random potential fluctuations, which corresponds to the white Gaussian noise potential, when exciton localisation takes place resulting in the low-energy shift of the exciton peak.

4. Conclusions

In this paper we have developed a semi-analytical quantum-mechanical description of the optical absorption spectrum for 2D-excitons in a rough QW taking into account the exciton localisation in the random potential fluctuations at the interface. The proposed method is based on the path-integral technique for calculating density of states in disordered systems. In this model the exciton c.o.m. motion near the interface in the field of the random individual scattering potentials, generated by local well-thickness fluctuations is considered. Gaussian statistics for the random distribution of the fluctuation potential is assumed. Asymptotic expressions for the low- and high-energy tails of the optical density function are obtained and alternative high-energy tail asymptotic using the perturbation theory is also presented. By using a nonlinear fitting procedure we have found an analytical interpolation function joining the two limiting asymptotics (for both cases under consideration) for any value of the variance of the random potential.

The calculated spectra exhibit the typical features observed in other methods of optical absorption calculations, such as the pronounced asymmetric shape, broadening of the excitonic line and apparent low-energy shift of the maximum. Using the fitting parameters to the time-resolved experiments [8] obtained in [6] a comparison between the FWHM inferred from fully path-integral calculations and the calculations using perturbation theory for the high-energy tail, has been performed. The comparison shows a much broader spectrum resulting from the fully path-integral approach with respect to the perturbation theory spectrum. This is due to the contribution of the localized exciton states in the high-energy tail of the spectrum, resulting from the semiclassical Kane tail in the density of states, which is absent within the perturbation theory approach since only the free-exciton states are taken into account there. In both cases under consideration we have found a logarithmic dependence of the FWHM on the variance of the random potential.

Our results for the effect of the variation of the correlation length on the optical density function are consistent in both classical and quantum limits, tending to the free-exciton peak at large correlation lengths and monotonically broadening in the quantum limit. The proposed method of calculation is relatively simple, since it uses analytical expressions for the optical density function across the whole energy range.

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Effect of random well-width fluctuations on the exciton optical absorption spectrum in single quantum wells

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The optical density function is calculated in a single quantum well for two-dimensional excitons moving in a random potential in the interfacial plane generated by fluctuations of the quantum-well thickness. Assuming Gaussian statistics for the random potential distribution, we have applied the path-integral approach and obtained in the adiabatic approximation two asymptotic analytical expressions for the low- and high-energy tails of the optical absorption spectrum. The high-energy tail of the exciton absorption line is also calculated using the perturbation theory. In order to obtain the spectrum across the whole energy range an analytical interpolation formula is found between the asymptotic expressions in the two cases, taking into account the proper normalization of the spectral function. The calculated optical density function is asymmetrically broadened, the magnitude of the peak is reduced, and the maximum is shifted to lower energy in both cases considered, as the disorder increases, in agreement with other theoretical results. Using the fitting parameters to the time-resolved photoluminescence data of Zimmermann [Nuovo Cimento D 17, 1801 (1995)], we find that the path-integral method leads to results for the spectral widths (full widths at half maximum) that are closer to those experimentally observable, as compared with results inferred from the perturbation theory approach. This can be attributed to the additional contribution of the localized exciton states from the Kane band tail in the former method. The effect of varying the correlation length (at a fixed depth of the random potential fluctuations) on the optical density function is also studied.

I. INTRODUCTION

The effect of in-plane interface disorder on the optical properties of two-dimensional (2D) excitons is currently being studied with renewed interest due to its persistence in both cw and time-resolved experiments. In narrow quantum wells (QW's) the interfacial disorder generates potential fluctuations resulting in band tails in the exciton density of states composed from localized states. Due to the static disorder the optical response of the Wannier excitons in QW's exhibits significant broadening and distinct asymmetry of the exciton line manifested by mixed Lorentz-Gaussian line shapes.[1] Modification of the exciton radiative lifetime and of the corresponding photoluminescence spectra is also predicted as a consequence of the presence of interfacial disorder and exciton localization.[2,3] In addition to the influence on the line shape, a substantial Stokes shift between the exciton lines in absorption and photoluminescence spectra is observed at low temperatures[4] due to interface roughness. These phenomena can be viewed as effects of dephasing, or partial breakdown of temporal coherence. As has been pointed out in Ref. 5, the static disorder by itself induces no dephasing since all scattering processes are elastic. On the other hand, since the disorder produces partial exciton localization (due to the band-tailing phenomenon) this in turn results in inhomogeneous distribution of the exciton energies. The incident pulse excites all oscillators in phase, but the excitons with different energies have different phases and they interfere with each other; this can be termed disorder-induced dephasing.

Disorder can also be considered as the origin of momentum broadening and resonant Rayleigh scattering.[6–8] The effects of the disorder and the exciton inhomogeneous broadening on time-resolved optical spectra are currently being extensively investigated (see, e.g., Ref. 5). Disorder is responsible for the finite rise time in the time-resolved behavior of secondary radiation (Rayleigh scattering and luminescence).[8–11] These phenomena imply scattering and partial breakdown of spatial coherence.

The microscopic origin of the interface disorder is related to interface roughness (steps or islands) and atomic interdiffusion, e.g., the cationic exchange in $GaAs/Al_xGa_{1-x}As$, which occurs for thermodynamical reasons and results in compositional fluctuations. We shall focus our attention on the statistical well-width fluctuations arising from local thickness fluctuations during crystal-growth processes. The Fourier spectrum of the interfacial roughness contains short- and long-wavelength components, the latter related to the atomically smooth growth islands (with lateral dimensions exceeding the exciton Bohr radius) separated by one-monolayer steps that have been experimentally observed in $GaAs/Al_xGa_{1-x}As$ quantum wells by the cathodoluminescence technique.[12] The photoluminescence spectrum is very sensitive to the size of the islands. For large enough islands

splitting of the exciton linewidth is observed (see Ref. 13 and references therein). However, in this paper we shall be interested in the small-island-size regime resulting in rapid interfacial fluctuations.

The classical treatment of exciton motion in a disorder interface potential is unable to explain the inhomogeneous broadening and consequent asymmetry of the exciton lines in 2D.[14,15] Early attempts at obtaining analytical closed-form descriptions of the exciton spectra in the presence of disorder within the quantum-mechanical theory were restricted to obtaining the spectral density function in one dimension with a specified type of statistical random potential distribution[16] (e.g., a white-Gaussian-noise potential). Most of the present theoretical studies are based on the solution of Schrödinger's equation for the exciton center-of-mass (c.m.) motion.[2,9,17,18] Within this approximation the assumption that the disorder does not affect the exciton internal degrees of freedom[2,9] has been made, which is fulfilled provided that the band-edge fluctuation amplitude along the QW plane is smaller than the exciton confinement energy. The latter represents a reasonable assumption, from the experimental point of view, since it is valid for high-quality samples. Zimmermann[9] solved the Schrödinger equation for the exciton c.m. motion in a random potential by considering an expansion of the potential fluctuations due to the variation of the well width up to lowest order using the transfer matrix method. The exciton optical density function in a one-dimensional Gaussian random potential (an exciton in a rough quantum wire) has been calculated using Dyson's integral equations for the probability densities.[19] The calculated spectra exhibit a distinct asymmetry and broadening, with the maximum shifted slightly to lower energies, which gives rise to dephasing. Generally, there are fundamental difficulties in solving the problem in 2D and the results in 1D are usually taken as a model for the asymmetric line shape of 2D QW excitons. However, it is likely that such a simplified approach is not be applicable[18] in modeling real 2D exciton spectra.

A quantum-mechanical theory of the influence of disorder on free-particle motion was developed in Ref. 17 using a Green's function expansion with respect to the Fourier transform of the binary correlation function of the random potential fluctuations. An analytical formula was derived for the asymmetrically broadened and shifted spectral function, and numerical calculations were performed for Gaussian fluctuations in 1D and 2D using the linear optical susceptibility. Another numerical method for optical absorption in quantum structures was proposed in Ref. 18. It is based on real-space representation of the Hamiltonian and time-dependent solution of the Schrödinger equation and calculation of the optical susceptibility as an initial-value problem. The method has been applied to excitons on rough interfaces and the calculated spectra show that the 1D model gives only a very rough approximation to the line shape in 2D.

The effect of inhomogeneous broadening on the exciton absorption line was studied with a semiclassical model in Ref. 5, where the exciton resonance frequency was assumed to have a Gaussian distribution. The absorption line shape of a single QW, within the framework of the linear nonlocal response theory was calculated for both homogeneous and inhomogeneous broadening in 1D, resulting in Gaussian tails of the inhomogeneous broadened spectrum. Since this represents a semiclassical treatment, only symmetric line shapes are produced.

The problem of the coupling of the relative and c.m. motions of the electron-hole pair by the disorder potential has been tackled by means of a Green's function theory approach to the optical response of disordered semiconductors proposed in Ref. 20. As an application calculation of the linear optical properties of a semiconductor QW with interface roughness was performed. Due to the anisotropy of the QW structure, the absorption spectrum depends on the angle of the incident light with respect to the QW plane. In order to account for the simultaneous influence of the propagation and disorder, Maxwell's equations were included in the analysis. The linear susceptibility was obtained from the configuration-averaged-polarization Green's function. The optical absorption spectra both parallel and perpendicular to the QW were calculated. An asymmetric shape and a slight redshift were found for the in-plane $1s$ excitonic resonance.

In this paper we aim to develop a semianalytical quantum-mechanical description of asymmetric exciton line shapes, line broadening, and low-energy shift of the optical absorption spectrum for 2D excitons in a QW, taking into account the exciton localization in the random potential fluctuations at the interface. The latter is achieved by applying the Feynman path-integral method for calculation of the band tail and semiclassical exciton density of states. Our approach will mainly follow Ref. 2, where two asymptotic expressions for the optical density function for the high- and low-energy tails of the absorption spectrum were obtained. The high-energy tail of the spectrum calculated in Ref. 2 was obtained using perturbation theory and the low-energy tail by the optimal fluctuation technique,[21,22] assuming a white-Gaussian-noise correlation function. Analytical interpolation formulas joining the two asymptotic expressions have been found for the optical absorption spectrum in the whole energy range.

In what follows, we shall show that such a semianalytical approach turns out to be more advantageous compared to the pure numerical computations in 2D,[18] and implies linewidths closer to those experimentally observed. In distinction from the method of Efros and Wetzel[2] we calculate the optical density function using the general path-integral 2D exciton density of states, assuming a Gaussian random potential distribution and a Gaussian binary correlation function. Our calculations are based on the expression for the 3D electron density of states that was derived by one of us[23] (V.S.) using the Feynman path-integral method and was further generalized for the d-dimensional case in Ref. 24. As limiting cases of the general path-integral expression for the exciton density of states in 2D, we have obtained the low- and high-energy tails of the optical absorption spectrum. Thus, in the high-energy limit, in contrast with Ref. 2, we account for the localized exciton states in the semiclassical Kane band tail,[25,26] which in turn contribute to the high-energy density of states and high-energy tail of the absorption spectrum. Interpolation between the two asymptotics has been performed for an optical density function depending on two variables (energy and the variance of the random potential), thus obtaining the full 3D profiles of the optical absorption as a function of the disorder (represented by the variance of the random potential fluctuations). Finally, a full 2D exciton

absorption spectrum calculation is performed. It should be noted that our path-integral approach differs from all other approaches by allowing us to treat on an adequate basis both the short- and long-range correlations in order to account for the whole spectrum of the fluctuating potential.

The outline of the paper is as follows. In Sec. II we describe the theoretical model and the analytical calculations, respectively, for the path-integral approach and the high-energy spectrum tail calculation using the alternative perturbation theory approach. In Sec. III numerical results for the calculated optical absorption spectra are presented, and the influence on the spectra of independently varying the two disorder parameters is studied. Comparison with time-resolved photoluminescence data is also made. Section IV contains concluding remarks.

II. THEORETICAL MODEL AND ANALYTICAL CALCULATIONS

A. Optical density function

We shall consider the motion of a 2D exciton in a random potential whose wave function according to Ref. 27 can be represented by the product

$$\Psi(\mathbf{r}_e,\mathbf{r}_h)=\Psi(\mathbf{R})\varphi(\rho)\chi_e(z_e)\chi_h(z_h), \tag{1}$$

where $\mathbf{r}_{e,h}(\rho_{e,h},z_{e,h})$ are the electron and hole coordinates, respectively in plane and perpendicular to the plane of a quantum well, $\rho=\rho_e-\rho_h$ is the coordinate of the relative motion of the two carriers, $\mathbf{R}=(m_e\rho_e+m_{h\parallel}\rho_h)/M$ is the exciton's c.m. coordinate, and $M=m_e+m_{h\parallel}$ is the total heavy-hole exciton mass, $m_e,m_{h\parallel}$ being the electron and heavy-hole masses parallel to the interface. $\Psi(\mathbf{R})$ is the exciton's c.m. wave function describing its motion in the quantum-well plane and $\chi_e(z_e)$ and $\chi_h(z_h)$ are the wave functions for electron and hole motion in the z direction (perpendicular to the interfacial plane), which for the electrons (or holes) only is that of a particle in a one-dimensional quantum well. $\varphi(\rho)$ is the exciton wave function describing the in-plane relative motion of the electron and hole, which in the pure 2D case is given by

$$\varphi(\rho)=\frac{4}{a_B^*\sqrt{2\pi}}e^{-2\rho/a_B^*},$$

where $a_B^*=\epsilon_s\hbar^2/\mu e^2$, ϵ_s is the semiconductor dielectric constant (assumed equal for both materials of the QW), and $\mu=m_em_h/M$ is the reduced effective mass.

Within the adiabatic approximation we shall assume that the exciton line is slightly broadened, i.e., the linewidth is smaller than for the 2D exciton binding energy and the energies of the electron and hole quantization along the z axis within the well. Therefore the solution for the exciton wave function can be factorized out and thus we end up with a Schrödinger equation for a particle of mass M in a random adiabatic potential:

$$\left[-\frac{\hbar^2\nabla^2}{2M}+V(\mathbf{R})\right]\psi(\mathbf{R})=E\psi(\mathbf{R}). \tag{2}$$

Our model is aiming to find the spectral function of a single particle (the exciton center of mass) in a field of N scatterers confined in an area S at the interface during its motion near the disordered interface of the quantum well obeying the Hamiltonian

$$\hat{H}=\hat{H}_0+V(\mathbf{R}), \tag{3}$$

where $\hat{H}_0$ is the unperturbed Hamiltonian of the ordered system without randomness and the random in-plane potential $V(\mathbf{R})=\Sigma_i v(\mathbf{R}-\mathbf{R}_{0i})$ (Fig. 1) is a superposition of individual scattering potentials $v(\mathbf{R}-\mathbf{R}_{0_i})$ representing the 2D random potential generated at a point $\mathbf{R}(x,y)$ in the heterojunction interfacial plane by the local well-width fluctuation located at $\mathbf{R}_{0i}(x_{0i},y_{0i})$ in the plane. The statistical properties of the random potential energy distribution are characterized by its moments. We shall assume a Gaussian statistical distribution, which is completely described by its first and second moments, i.e., by the mean potential energy and the binary correlation function:

$$E_0=\langle V(\mathbf{R})\rangle=\bar{N}_{2D}\int d\mathbf{R}_0 v(\mathbf{R}-\mathbf{R}_0), \tag{4}$$

$$\begin{aligned}W(\mathbf{R}-\mathbf{R}')&=\langle V(\mathbf{R})V(\mathbf{R}')\rangle\\&=\bar{N}_{2D}\int d\mathbf{R}_0 v(\mathbf{R}-\mathbf{R}_0)v(\mathbf{R}'-\mathbf{R}_0)\\&=\xi_L e^{-|\mathbf{R}-\mathbf{R}'|^2/L^2},\end{aligned} \tag{5}$$

where $\bar{N}_{2D}=N/S$ is the surface density of the scattering centers, L is the correlation length of the random potential fluctuations, and ξ_L is the variance of the random Gaussian po-

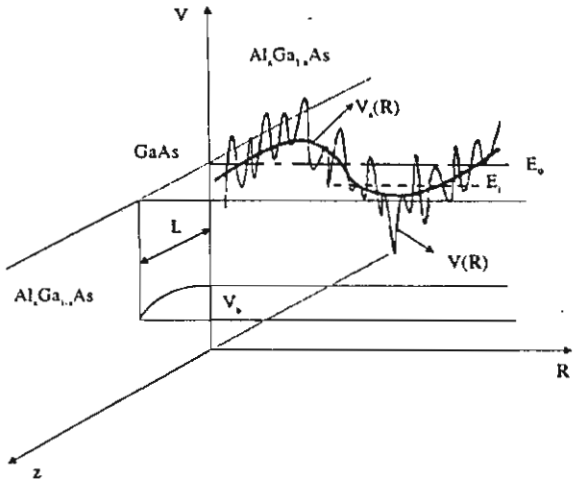

FIG. 1. Plot of the random potential $V(\mathbf{R})$ experienced by the exciton c.m. in the interfacial plane of a single quantum well ($\mathbf{R}$ is the 2D in-plane c.m. coordinate) varying about the average potential of the random system E_0. Along the z axis perpendicular to the interfacial plane the alternating layers of $Al_xGa_{1-x}As$ and GaAs are represented, showing the potential profile of the quantum well (L being the width and V_b the quantum-well depth). The smoothed potential over the characteristic size of the exciton c.m. envelope wave function (Ref. 29) $V_s(\mathbf{R})$ is also represented; E_j is a local low-energy level of the exciton c.m., localized in the minimum of the smoothed potential.

tential. The quantity ξ_L, having the dimension of energy squared, was first introduced by Halperin and Lax[29] and represents a measure for the depth of the typical potential well. In the 2D case ξ_L is given by

$$\xi_L = \bar{N}_{2D}\left(\frac{\pi L^2}{4}\right) v_0^2. \tag{6}$$

In this expression we have introduced the strength (or amplitude) v_0 of the individual scattering potentials according to

$$v(\mathbf{R}-\mathbf{R}_0) = v_0 e^{-|\mathbf{R}-\mathbf{R}_0|^2/l^2} \tag{7}$$

and $L = l\sqrt{2}$.

The spectral density function for a 2D Schrödinger particle in a random potential is defined according to Ref. 16 by

$$A(\mathbf{K}_\parallel, E) = \frac{1}{S}\left\langle \sum_i \left| \int e^{i\mathbf{K}_\parallel \cdot \mathbf{R}} \Psi_i(\mathbf{R}) d\mathbf{R} \right|^2 \delta(E-E_i) \right\rangle, \tag{8}$$

where $\Psi_i(\mathbf{R})$ is the center-of-mass wave function of the ith exciton state with a corresponding energy E_i, $\mathbf{K}_\parallel$ is the 2D exciton wave vector in the plane parallel to the interface, and S is the normalization area. The above averaging is performed over all possible configurations of the random potential fluctuations ($\langle \cdots \rangle$ indicating an average over the statistical ensemble).

Since we shall be interested in the optical absorption spectrum, we wish to calculate the optical density function that represents the $\mathbf{K}_\parallel = 0$ value of the spectral density Eq. (8):

$$A(E) = \frac{1}{S}\left\langle \sum_i \left| \int d\mathbf{R} \Psi_i(\mathbf{R}) \right|^2 \delta(E-E_i) \right\rangle. \tag{9}$$

Then the absorption coefficient can be written as

$$\alpha(\omega) = \alpha_0 A(E), \tag{10}$$

where α_0 is a slowly varying function of the excitation frequency ω (see, e.g., Ref. 28).

B. Path-integral approach for calculation of the optical density function

In order to calculate the optical density function we need to obtain the 2D excitonic density of states (DOS). Reformulating the problem in path-integral (PI) terms, we need to calculate the average (over all random potential configurations) exciton one-particle propagator

$$\bar{G}(\mathbf{R}_2, \mathbf{R}_1; t) = \int D[\mathbf{R}(\tau)] e^{iS/\hbar} \tag{11}$$

satisfying the boundary conditions $\mathbf{R}(0) = \mathbf{R}_1$, $\mathbf{R}(t) = \mathbf{R}_2$, where S is the action of the random system, resulting from the averaging over all impurity configurations. S is given up to the second-order moment of the random potential distribution by

$$S = \int_0^t d\tau \left(\frac{M}{2}\dot{\mathbf{R}}^2(\tau) - E_0 + \frac{i}{2\hbar}\int_0^t d\sigma\, W[\mathbf{R}(\tau)-\mathbf{R}(\sigma)] \right). \tag{12}$$

The density of states per unit area is given by the Fourier transform of the diagonal part of the configurationally averaged one-particle propagator:

$$\rho(E) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt\, e^{iEt/\hbar}\bar{G}(0,0;t). \tag{13}$$

Therefore the problem of a density of states calculation within the framework of the path-integral approach consists in evaluating the exact propagator by integrating over all possible paths using S. As was initially pointed out in Ref. 23, this step can be approximated by introducing a trial action S_0 based on the harmonic oscillator potential to average the relevant variables over paths. The perturbation $S - S_0$ is then calculated using these approximate averages. This procedure is analogous to the use of a "universal wave function" by Halperin and Lax.[29] The harmonic oscillator potential is equivalent to modeling the real wave function by a quadratic function (Gaussian). The use of a harmonic trial action is equivalent to assuming that all the fluctuating potentials have the same quadratic shape. Thus the problem of the density of states calculation becomes exactly solvable if the full action is approximated by a nonlocal harmonic oscillator "trial" action of the following form:

$$S_0 = \int_0^t d\tau \left(\frac{M}{2}\dot{\mathbf{R}}^2(\tau) - \frac{\Omega^2}{2t}\int_0^t d\sigma |\mathbf{R}(\tau)-\mathbf{R}(\sigma)|^2 \right). \tag{14}$$

The nonlocality of the trial action means that the harmonic oscillator can be anywhere in space. The nonlocal harmonic oscillator frequency Ω is used as a variational parameter to be adjusted as a function of energy subject to a variational principle.

The average propagator can be rewritten in terms of the trial action, using the path-integral normalization, the trial action introduced above corresponding to a zero-order approximation $\bar{G}_0$ to $\bar{G}$. By keeping only the first-order term in the cumulant expansion, a first-cumulant approximation $\bar{G}_1$ to $\bar{G}$ is obtained (see Refs. 30 and 31 for details), whose diagonal elements give the density of states (within the first-cumulant approximation).

The DOS per unit volume in the first-cumulant approximation for a Gaussian random potential with a Gaussian binary correlation function was derived in Ref. 23 and generalized in Ref. 24 for the case of a d-dimensional system:

$$\rho_1(E) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt \left(\frac{M}{2\pi i\hbar t}\right)^{d/2}\left(\frac{\Omega t}{2\sin \Omega t/2}\right)^d \times \exp\left[\frac{d}{2}\left(\frac{\Omega t}{2}\cot\frac{\Omega t}{2} - 1\right) - \frac{1}{2\hbar^2}\xi_L t\int_0^t dx\, j(x,\Omega)^{-d/2} + \frac{i}{\hbar}(E-E_0)t\right] \tag{15}$$

where Ω is a variational parameter to be determined and the function $j(x,\Omega)$ is given by

$$j(x,\Omega)=\left(1+\frac{i\hbar}{M\Omega}\frac{4}{L^2}\frac{\sin\Omega x/2\sin[\Omega(t-x)]/2}{\sin Qt/2}\right)$$
$$=\left(1+8i\frac{E_L}{E_\Omega}\frac{\sin\Omega x/2\sin[\Omega(t-x)]/2}{\sin\Omega t/2}\right) \quad (16)$$

where

$$E_\Omega=\hbar\Omega \text{ and } E_L=\hbar^2/2ML^2 \quad (17)$$

is the correlation energy (the kinetic energy of localization over a distance L, the correlation length of the random potential fluctuations), representing a measure of the exciton confinement. It has been previously shown[32] that in a small-time approximation the expression for the propagator [equivalent to retaining only high-exciton-energy states in $\rho_1(E)$ and physically understood by considering the "pseudo" Heisenberg uncertainty relation $Et\geq\hbar$] leads to Thomas-Fermi semiclassical results while a large-t approximation reproduces the results of Halperin and Lax[29] deep in the band tail.

Two limiting cases of energies in the band tail can be considered. At large negative energies deep in the band tail ($E-E_0\rightarrow-\infty$), the so-called "quantum case" is valid, for which the following condition is satisfied: $\lambda\gg L$, where $\lambda=\hbar/(2M\sqrt{\xi_L})^{1/2}$ is the Broglie wavelength of the free exciton and L is the correlation length, i.e., there are no exciton states in a region with the size of the characteristic potential well. The other limiting case ($|E-E_0|\rightarrow\infty$) corresponds to a "classical well" containing many exciton states (i.e., $\lambda\ll L$). Therefore two analytical asymptotic expressions for the 2D exciton DOS ($d=2$) can be obtained from the above general expression in the so-called low-energy limit, i.e., deep in the excitonic band tail, and in the opposite extreme of high energy, i.e., near the band edge.

1. Low-energy limit

We shall be interested in calculating the optical density function for $\mathbf{K}_\parallel=0$ in the low-energy tail, i.e., the region of large negative energies below the unperturbed band edge. In what follows we shall apply the path-integral approach for 2D DOS calculations in the presence of a disorder potential[23] in determining the low-energy tail of the spectral function.

Let us consider first the DOS calculation in the excitonic band tail. As has been discussed in the previous section, in order to evaluate the ground-state energy contribution to the DOS, the limit $t\rightarrow\infty$ of the integrand in the general DOS expression[23,33] (15) is taken. The 2D exciton DOS deep in the band tail is obtained from that limit, by letting $E\rightarrow-\infty$. Introducing the dimensionless variational parameter $z=E_\Omega/E_L$ and energy normalizing with respect to the correlation energy according to

$$\nu=\frac{E_0-E}{E_L} \quad (18)$$

the following expression in 2D is obtained:

$$\rho_T(\nu)=\left[\left(\frac{E_L}{L}\right)^2\Big/\,\xi_L^{3/2}\right]a(\nu,z)e^{-E_b^2(\nu,z)/2\xi_L}, \quad (19)$$

where the preexponential factor and the factor in the exponent are obtained analogously to the 3D derivation[33] and are given by

$$a(\nu,z)=\frac{1}{2^{5/2}\pi^{3/2}}z^{1/2}(z+4)^{3/2}\left(\frac{z}{2}+\nu\right), \quad (20)$$

$$b(\nu,z)=\left(\frac{z}{2}+\nu\right)^2\left(1+\frac{4}{z}\right). \quad (21)$$

In order to obtain the variational parameter z we need to minimize the DOS exponent according to Ref. 29, which in turn leads to the following quadratic equation in the 2D case considered:

$$z^2+2z-4\nu=0. \quad (22)$$

Keeping only the positive root

$$z=\sqrt{1+4\nu}-1, \quad (23)$$

which has physical meaning, and substituting it into Eqs. (20) and (21), we obtain

$$a(\nu)=\frac{(\sqrt{1+4\nu}-1)^{3/2}(\sqrt{1+4\nu}+3)^{5/2}}{2^{9/2}\pi^{3/2}}, \quad (24)$$

$$b(\nu)=\frac{1}{2^4}(\sqrt{1+4\nu}-1)(\sqrt{1+4\nu}+3)^3. \quad (25)$$

Introducing the dimenensionless quantity

$$\xi'=\frac{\xi_L}{E_L^2}, \quad (26)$$

we obtain for the 2D DOS deep in the excitonic band tail

$$\rho_T(\nu)=\left(\frac{1}{E_LL^2}\frac{1}{\xi'^{3/2}}\right)a(\nu)e^{-b(\nu)/2\xi'}. \quad (27)$$

In order to calculate the optical density function, we rewrite Eq. (9) in the form of a functional integral over all possible potential fluctuations:

$$A(E)=\frac{1}{S}\int DV\,W(V)\sum_i\left|\int d\mathbf{R}\Psi_i(\mathbf{R})\right|^2\delta(E-E_i), \quad (28)$$

where $W(V)$ is the probability of the random potential distribution. The excitonic states deep in the low-energy tail are produced by deep and narrow random potential fluctuations and therefore the energy distance between the ground state and the excited states of the well is greater. Therefore the contribution of the excited states can be neglected deep in the band tail. In the low-energy range ($(E-E_0)/E_L\rightarrow-\infty$, or, equivalently, $\nu\gg1$) we shall be interested only in the ground-state contribution to the density of states (since we have taken the limit $t\rightarrow\infty$ in obtaining it), and we can consider that the main contribution to the above integral comes from the ground-state exciton center-of-mass wave function in a harmonic potential well, i.e.,

$$\Psi_0(\mathbf{R})=\left(\frac{2\gamma}{\pi}\right)^{1/2}e^{-\gamma R^2}, \quad (29)$$

where

$$\gamma=\frac{M\Omega}{\hbar}=\frac{z}{2L^2} \tag{30}$$

and z is a variational parameter, the same as that appearing in the band-tail DOS, and is given by Eq. (23). Therefore we can take the factor $|\int d\mathbf{R}\Psi_0(\mathbf{R})|^2$ out of the functional integral. The remaining functional integral is, by definition, the band-tail density of states $\rho_T(\nu)$. Therefore

$$A(E)=\left|\int d\mathbf{R}\Psi_0(\mathbf{R})\right|^2\rho_T(E)=\left(\frac{2\pi}{\gamma}\right)\rho_T(E). \tag{31}$$

Substituting γ and z from Eqs. (30) and Eq. (23) we obtain the following expression for the low-energy tail of the optical density function:

$$A(\nu)=\frac{4\pi L^2}{(\sqrt{1+4\nu}-1)}\rho_T(\nu). \tag{32}$$

2. *High-energy limit*

Let us consider now the calculation of the high-energy tail of the optical density function. In order to obtain the high-energy semiclassical Kane limit of the general PI expression for the 2D exciton DOS near the band edge, it is necessary to take the limit $t\to 0$ of the integrand of Eq. (15), which corresponds to retaining only high-energy excitonic states in the DOS. Taking into account that $\lim_{t\to 0} j(x,\omega)=1$, after integration over t this gives

$$\rho_K(E)=\frac{1}{2^{5/2}\pi^{3/2}E_L L^2}e^{(E_0-E)^2/4\xi_L}D_{-1}\left(\frac{E_0-E}{\sqrt{\xi_L}}\right), \tag{33}$$

where D_{-1} is the parabolic cylinder function of order -1. Finally, introducing dimensionless variables ξ' and ν we get

$$\rho_K(\nu)=\frac{1}{2^{5/2}\pi^{3/2}E_L L^2}e^{-\nu^2/4\xi'}D_{-1}\left(\frac{\nu}{\sqrt{\xi'}}\right). \tag{34}$$

In the opposite extreme, at high enough energies, the problem of finding the proper variational exciton wave function is not a straightforward one, since the high-energy states are described by noncompact fractal-shaped wave functions[38] and the corresponding optical absorption spectrum results from many small contributions due to those states. However, it is clear that the exciton c.m. wave functions $\Psi_i(\mathbf{R})$ have to be close to plane waves. According to Ref. 34, the exciton states close to the delocalized states can be described quite satisfactorily by choosing a c.m. envelope wave function of the form

$$\Psi_i(\mathbf{R})=A_0 e^{i\mathbf{K}_i\cdot\mathbf{R}-\gamma R^2},\quad A_0=\left(\frac{2\gamma}{\pi}\right)^{1/2}. \tag{35}$$

We shall consider that the main contribution to the configurational average in Eq. (9) at high energies is given by states with an equal shape of the envelope wave function, namely, Eq. (35). In what follows, we shall show that this particular choice of the envelope wave function results in realistic optical absorption spectra.

As in the first case (deep in the band tail) we can take the matrix element out of the ensemble averaging and the remaining average gives the semiclassical Kane 2D exciton DOS, Eq. (33).

The matrix element can be directly calculated, yielding

$$\left|\int d\mathbf{R}\Psi_i(\mathbf{R})\right|^2=\left(\frac{2\pi}{\gamma}\right)e^{-K_i^4/16\gamma^2}. \tag{36}$$

Therefore

$$A(E)=\left(\frac{2\pi}{\gamma}\right)e^{-K_i^4/16\gamma^2}\rho_K(E). \tag{37}$$

Substituting $K_i^2=2M(E_{K_i}-E_0)/\hbar^2$ and introducing the dimensionless energy according to Eq. (18), we obtain

$$A(\nu)=\left(\frac{2\pi}{\gamma}\right)e^{-\nu^2/16\gamma^2L^4}\rho_K(\nu), \tag{38}$$

where the semiclassical 2D exciton DOS is given by Eq. (29).

Finally, we obtain the following general expression for the optical density function at high energies:

$$A(\nu)=\frac{1}{2^{3/2}\sqrt{\pi}}\frac{1}{\gamma L^2 E_L}\times\exp\left[-\nu^2\left(\frac{1}{(4\gamma L^2)}+\frac{1}{4\xi'}\right)\right]D_{-1}\left(\frac{\nu}{\sqrt{\xi'}}\right). \tag{39}$$

In order to obtain the semiclassical Kane band tail we take the limit $|E-E_0|\to\infty$, i.e., $(E-E_0)/\sqrt{\xi_L}\ll -1$ or $\nu/\sqrt{\xi'}\gg 1$, and taking into account the asymptotic behavior of the parabolic cylinder function for large argument values, namely, $\lim_{z\to\infty} D_p(z)\sim e^{-z^2/4}z^p$, we obtain

$$A(\nu)=\frac{1}{2\sqrt{2\pi}}\frac{\sqrt{\xi'}}{\gamma L^2}\frac{1}{\nu E_L}\exp\left[-\nu^2\left(\frac{1}{(4\gamma L^2)^2}+\frac{1}{2\xi'}\right)\right]. \tag{40}$$

The opposite extreme, $E-E_0>0$, $E-E_0\to\infty$, i.e., $(E-E_0)/\sqrt{\xi_L}\gg 1$, $\nu/\sqrt{\xi'}\ll 1$, yields the free-exciton (continuum exciton states) 2D DOS (see, e.g., Ref. 35)

$$\rho^{sc}(\nu)=\frac{M}{2\pi\hbar^2}\left[1+\mathrm{erf}\left(\frac{\nu}{\sqrt{\xi'}}\right)\right]. \tag{41}$$

Therefore, the optical density function acquires the form

$$A(\nu)=\frac{1}{2\gamma L^2 E_L}\left[1+\mathrm{erf}\left(\frac{\nu}{\sqrt{\xi'}}\right)\right]e^{-\nu^2/(4\gamma L^2)^2}. \tag{42}$$

Finally, we obtain the following two limiting cases:

$$A(\nu)=\begin{cases}\dfrac{1}{2\sqrt{2\pi}}\dfrac{\sqrt{\xi'}}{\gamma L^2 E_L}\dfrac{1}{\nu}\exp\left[-\nu^2\left(\dfrac{1}{(4\gamma L^2)^2}+\dfrac{1}{2\xi'}\right)\right], & \dfrac{\nu}{\sqrt{\xi'}}\gg 1\\ \dfrac{1}{2\gamma L^2 E_L}\left[1+\mathrm{erf}\left(\dfrac{\nu}{\sqrt{\xi'}}\right)\right]e^{-\nu^2/(4\gamma L^2)^2}, & \dfrac{\nu}{\sqrt{\xi'}}\ll 1.\end{cases} \tag{43}$$

If we take the limit $\nu\to\infty$ of the free-exciton DOS [second line of Eq. (43)], since for the free excitons the difference between the energy of the exciton c.m. and the mean potential energy E_0 is expected to be much larger than the localization energy E_L, we obtain a pure Gaussian exciton line shape:

$$A(\nu)=\frac{1}{\gamma L^2 E_L}e^{-\nu^2/(4\gamma L^2)}. \tag{44}$$

The dimensionless parameter $\gamma L^2=z/2$ in Eq. (43) depends on the variational parameter z introduced in the calculation procedure for the low-energy tail of the spectral density and is given by Eq. (23).

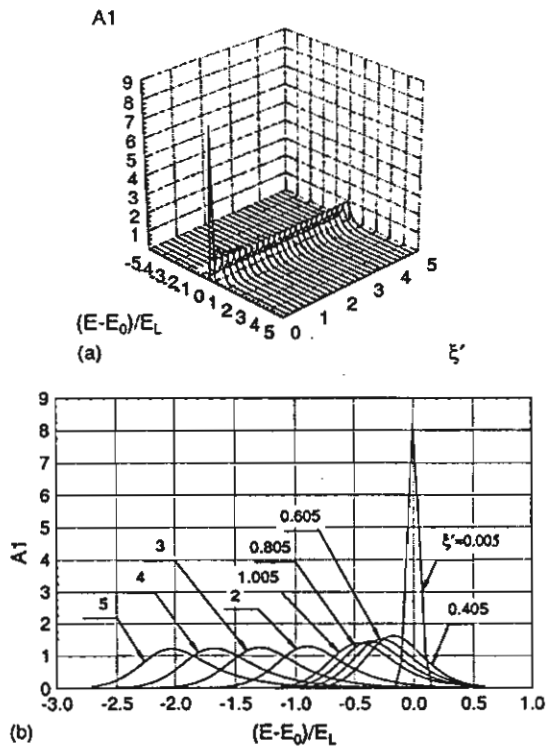

FIG. 2. Plot of the normalized optical density function vs dimensionless energy $(E-E_0)/E_L$ and dimensionless disorder parameter ξ' calculated on the basis of the perturbation theory high- and low-energy tails, inferred from the path-integral approach (referred to as case 1 in the text). (a) 3D trace plot; (b) cross sections of (a) at $\xi'=0.005,0.405,0.605,0.805,1.005,2,3,4,5$. The correlation energy has been kept constant at $E_L=0.12$ meV.

C. Perturbation theory approach for high-energy tail of the optical density function

One might expect that the high-energy behavior of the optical absorption spectrum at very weak disorder would be limited by the perturbation theory results accounting for delocalized states in the spectrum. In order to check this, let us calculate the high-energy tail of $A(E)$ using perturbation theory. In this region the exciton center-of-mass envelope wave functions are nearly plane waves.

Using the perturbation theory in the high-energy limit, we have

$$A(E)=\frac{1}{S}\int\frac{d^2K_\parallel}{(2\pi)^2}\frac{\langle|\int V(\mathbf{R})e^{i\mathbf{K}_\parallel\cdot\mathbf{R}}d\mathbf{R}|^2\rangle}{E^2_{K_\parallel}}\delta(E-E_{K_\parallel}). \tag{45}$$

Let us first calculate the average:

$$\left\langle\left|\int V(\mathbf{R})e^{i\mathbf{K}_\parallel\cdot\mathbf{R}}d\mathbf{R}\right|^2\right\rangle=\int d\mathbf{R}\int d\mathbf{R}'e^{i\mathbf{K}_\parallel\cdot(\mathbf{R}-\mathbf{R}')}\times\langle V(\mathbf{R})V(\mathbf{R}')\rangle. \tag{46}$$

Substituting the correlation function $\langle V(\mathbf{R})V(\mathbf{R}')\rangle$ from Eq. (5) and performing the integration by introducing the new variable $\mathbf{x}=\mathbf{R}-\mathbf{R}'$ (because of the translational invariance in the plane parallel to the interface), we obtain

$$\left\langle\left|\int V(\mathbf{R})e^{i\mathbf{K}_\parallel\cdot\mathbf{R}}d\mathbf{R}\right|^2\right\rangle=\xi_L S\pi L^2 e^{-K_\parallel^2L^2/4}. \tag{47}$$

After performing the integration over the 2D in-plane wave vector in Eq. (45), finally we obtain the following expression:

$$A(E)=\frac{\xi_L ML^2}{2\hbar^2}\frac{e^{-(2ML^2/4\hbar^2)E}}{E^2}. \tag{48}$$

Introducing the dimensionless energy according to Eq. (18) and the dimensionless parameter ξ' according to Eq. (26) we can rewrite it as

$$A(\nu)=\frac{\xi'}{4E_L\nu^2}e^{-\nu/4}. \tag{49}$$

Comparing Eq. (49) with the path-integral expression (44) at high energies, we can conclude that (for strong enough disorder) the perturbation theory result for the high-energy shoulder of the spectrum decays faster than the semiclassical limit of the path-integral result, resulting in a broader spectrum. As will be shown in Sec. III, for weak disorder the high-energy side of the spectrum tends to the perturbation theory results, while on increasing the disorder the departure of the path-integral result from that of the perturbation theory becomes increasingly pronounced.

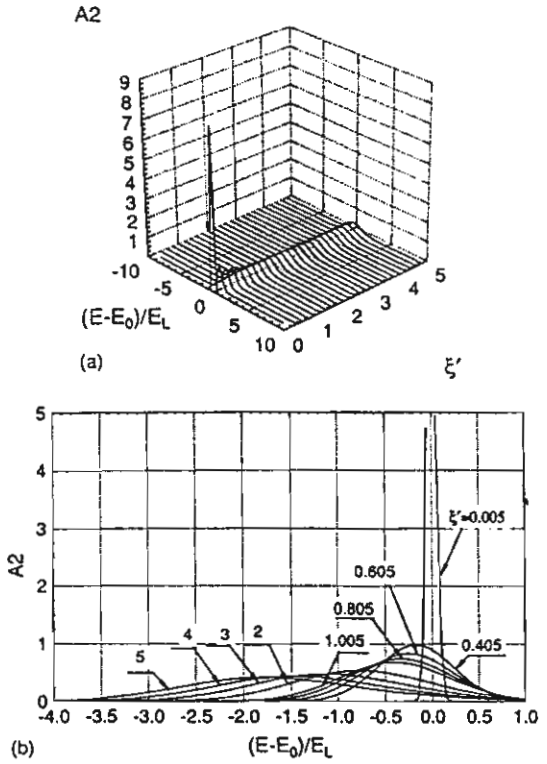

FIG. 3. Plot of the normalized optical density function vs dimensionless energy $(E-E_0)/E_L$ and dimensionless disorder parameter ξ' calculated using the path-integral method for both the high- and low-energy tails of the spectrum (referred to as case 2 in the text). (a) 3D trace plot; (b) cross sections of (a) at $\xi'=0.005,0.405,0.605,0.805,1.005,2,3,4,5$. The correlation energy has been kept constant at $E_L=0.12$ meV.

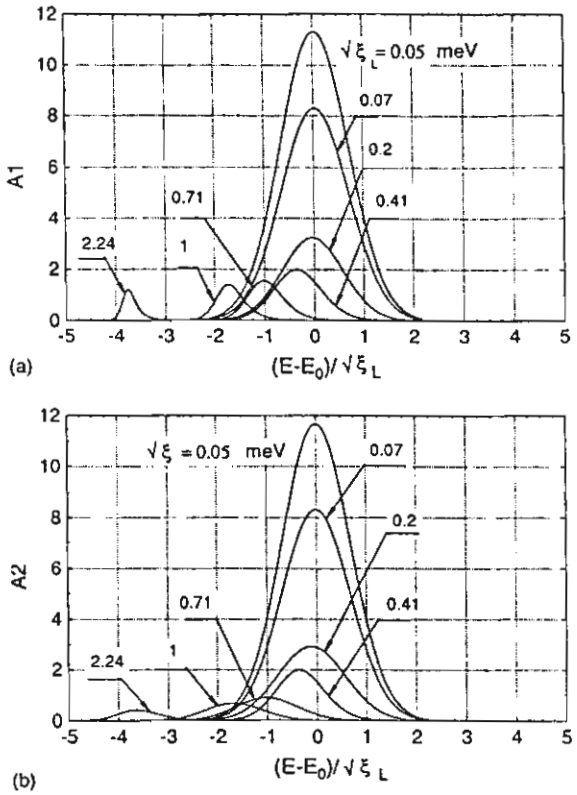

FIG. 4. (a) Plot of the optical density function corresponding to case 1 vs energy, normalized with respect to the standard deviation of the random potential $\sqrt{\xi_L}$: a measure for the magnitude of the potential fluctuations for different values of the standard deviation $\sqrt{\xi_L}=0.05,0.07,0.2,0.41,0.71,1,2.24$ meV; the low-energy shift of the maximum is clearly seen. The plots are calculated assuming a constant correlation energy $E_L=0.12$ meV. (b) Plot of the optical density function corresponding to case 2 vs energy, normalized with respect to the standard deviation of the random potential $\sqrt{\xi_L}$ for different values of the standard deviation $\sqrt{\xi_L}=0.05,0.07,0.2,0.41,0.71,1,2.24$ meV (all the plots are at $E_L=0.12$ meV).

III. NUMERICAL COMPUTATIONS AND RESULTS

In Sec. II we have obtained using a path-integral method low-energy [given by Eqs. (32), (27), (24), and (25)], and high-energy [Eq. (39)] asymptotic expressions for the optical density function and an alternative high-energy asymptotics resulting from the perturbation theory [Eq. (49)]. Since we are interested in the spectrum across the whole energy range, an interpolation function between Eqs. (32) and (49), hereinafter referred to as case 1, and also between Eqs. (32) and Eq. (39), referred to as case 2, has to be sought. The interpolation function in both cases has been found by performing a nonlinear fitting procedure based on the χ^2 minimization criterion. Using the proper normalization condition for the optical density function fulfilled for any value of the disorder parameter ξ',

$$\int_{-\infty}^{\infty} A(\nu,\xi')\,d\nu=1, \tag{50}$$

we obtain the following normalized interpolation functions:

$$A(\nu,\xi')=\begin{cases}\dfrac{\xi' e^{-1.039\,75\nu/\xi'}(0.536\,65\nu^2+1.358\,51\nu+0.819\,27)}{(\nu^2+0.285\,51)^2\left[4.216\,14\sqrt{\xi'}+10.013\,00e^{0.296\,863/\xi'}(\xi'-0.406\,64)\operatorname{erfc}\left(\dfrac{0.544\,85}{\sqrt{\xi'}}\right)\right]}, & \text{case 1}\\[2ex] \dfrac{0.238\,10e^{-2.830\,76/\xi'}}{\operatorname{erfc}\left(\dfrac{1.682\,49}{\sqrt{\xi'}}\right)}\dfrac{e^{-1.06\,50\nu^2/\xi'}(\nu+2.180\,72)}{\nu^2+2.666\,78}, & \text{case 2}\end{cases} \tag{51}$$

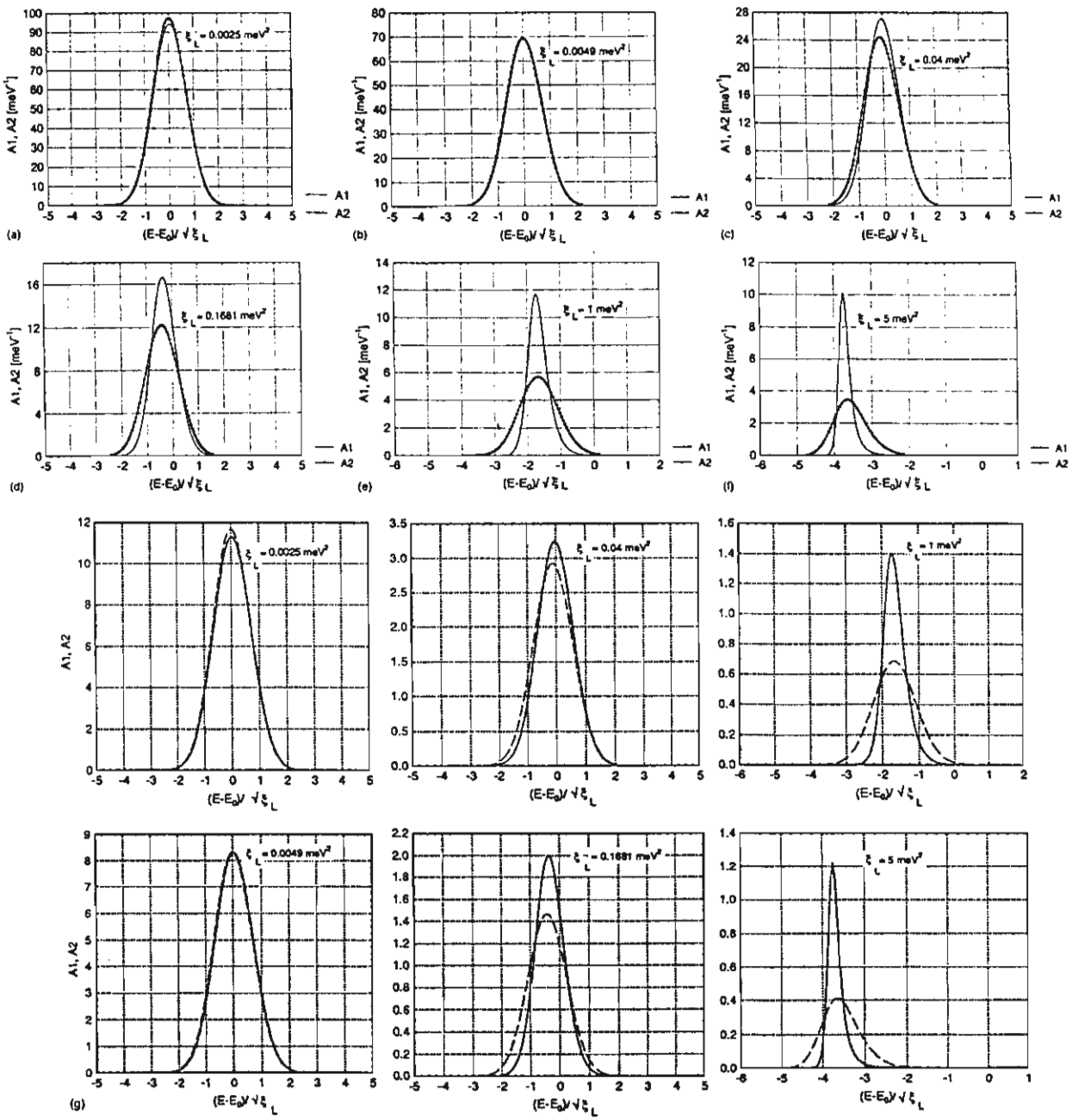

FIG. 5. Plot of the optical density functions corresponding to case 1 (A1, solid line) and case 2 (A2, dashed line) as a function of the normalized energy with respect to the standard deviation of the random potential fluctuations at different values of the variance: ξ_L = 0.0025,0.0049,0.04,0.1681,1,25 meV^2 (all the plots are at E_L=0.12 meV).

In Figs. 2(a), 2(b), and 3(a) and 3(b) the 3D trace plots of the normalized optical density from Eq. (50) as a function of the dimensionless energy with varying disorder parameter are shown for the first and the second cases, respectively. The spectra have been multiplied by the correlation energy in order to render them dimensionless. The exciton absorption line influenced by the random potential in both cases exhibits (i) a distinct asymmetry of the high- and low-energy shoulders of the spectrum with respect to the peak value, (ii) monotonic broadening and decrease of the magnitude of the exciton peak with increasing disorder, and (iii) shift of the maximum to lower energies. The redshift is clearly seen in Figs. 4(a) and 4(b) (for the first and second cases, respectively) where the optical density function is plotted against the energy in meV normalized with respect to the rms value of the amplitude of the random potential fluctuations $\sqrt{\xi_L}$ while the disorder parameter ξ_L is varied. On increasing the standard deviation of the random potential fluctuations about the mean, the exciton absorption line broadens, the intensity of the spectrum decreases, and the peak shifts to lower ener-

gies. The observed low-energy shift of the exciton peak with the disorder parameter (representing a measure of the depth of the random potential fluctuations) results from the fact that an increasingly greater part of the excitons becomes localized in the minima of the potential relief with an energy below the unperturbed band edge. The maximum of the excitonic energy distribution is centered at an energy corresponding to the exciton absorption peak. These results are consistent with previously calculated absorption spectra, e.g., the numerical calculation using the Green's function expansion applied in the one-dimensional case,[17] and with results of Zimmermann[9] and linear response theory results.[20] From the figures it can be clearly seen that on reducing the disorder parameter the shape of the spectral line approaches a δ-like free-exciton peak (in agreement with the expected δ-shaped free-exciton spectrum). This confirms the ability of the method to correctly obtain the free-exciton limit at zero disorder. Another feature of the calculated optical density spectrum is the sharp decrease of its intensity below $\xi' \sim 1$ [see Figs. 2(a) and 3(a)], i.e., for standard deviations of the random potential energy about its mean value of the order of the correlation energy E_L. Above the correlation energy the decrease of the magnitude of the exciton's peak is negligible and it remains almost constant up to very high values of ξ'. This behavior can be explained by smoothing of the potential fluctuations with a characteristic length greater than the correlation length L.

In order to confirm the limiting behavior of the optical absorption spectrum with the perturbation theory results for weak disorder, we have plotted both high-energy spectra with the same path-integral low-energy side in Fig. 5 at different values of the disorder parameter (variance of the random potential fluctuations) ξ_L. As can be seen there exists a range of disorder up to ~ 0.05 meV^2 where both approaches tend to the same high-energy tail; thus we can establish the limit of applicability of perturbation theory. Above this value the perturbations cannot be considered as small and the perturbation theory ceases to be valid.

In order to evaluate typical values of the full width at half maximum (FWHM) inferred from the calculated spectra we have taken the heavy-hole standard deviation and correlation energy values, namely, $\sqrt{\xi_L}=0.41$ and $E_L=0.12$ meV, obtained in Ref. 7 by fitting the time-resolved photoluminescence data of Wang *et al.*[10] The calculated optical absorption spectra are shown for two values of the variance, $\sqrt{\xi_L}=0.41$ and 1 meV in Figs. 6(a) and 6(b) and 7(a) and 7(b) (corresponding to the first and second cases considered, respectively). The problem of determining the energy zero of

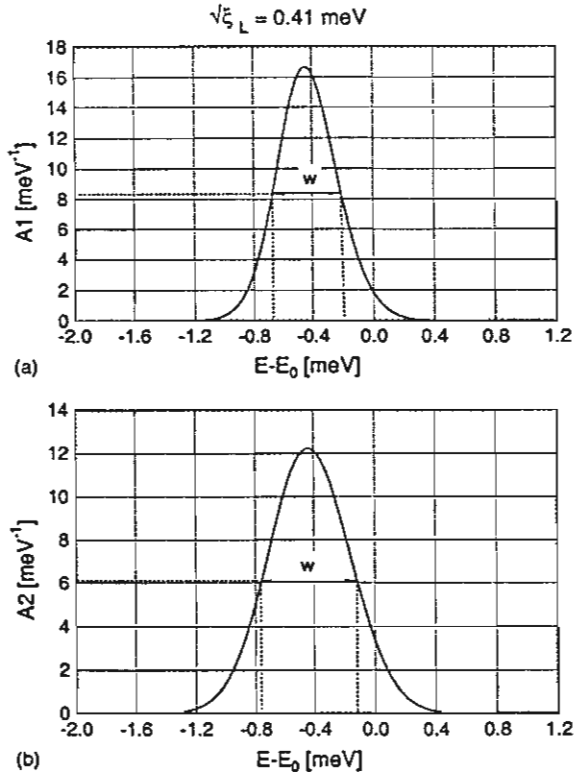

FIG. 6. (a) Optical density function calculated with the perturbation theory result for the high-energy tail and path-integral result for the low-energy tail of the spectrum (corresponding to case 1) vs energy at $\sqrt{\xi_L}=0.41$ meV. The FWHM is denoted by w (E_L is kept constant at 0.12 meV). (b) Optical density function calculated with the path-integral result for both high- and low-energy tails of the spectrum (corresponding to case 2) vs energy at $\sqrt{\xi_L}=0.41$ meV. The FWHM is denoted by w (E_L is kept constant at 0.12 meV).

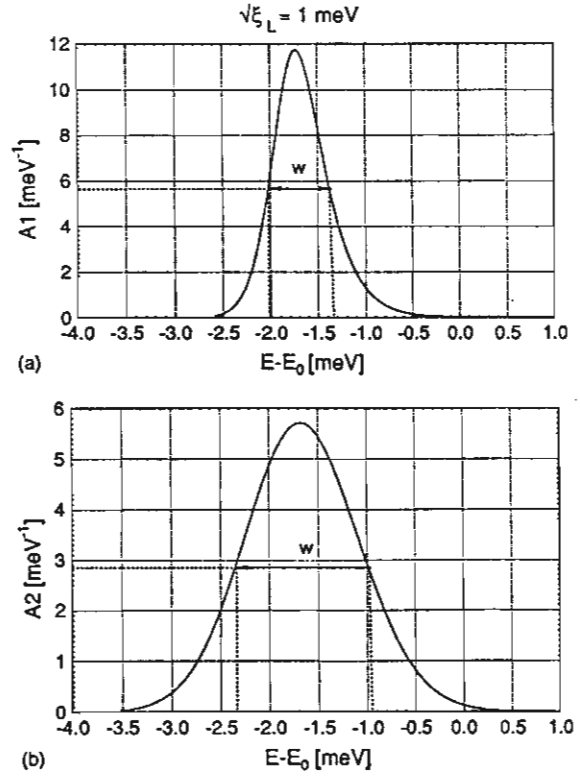

FIG. 7. (a) Optical density function calculated with the perturbation theory result for the high- energy tail and path-integral result for the low-energy tail of the spectrum (corresponding to case 1) vs energy at $\sqrt{\xi_L}=1$ meV (at a constant correlation energy $E_L=0.12$ meV). (b) Optical density function calculated with the path-integral result for both high- and low-energy tails of the spectrum (corresponding to case 2) vs energy at $\sqrt{\xi_L}=1$ meV (at a constant correlation energy $E_L=0.12$ meV).

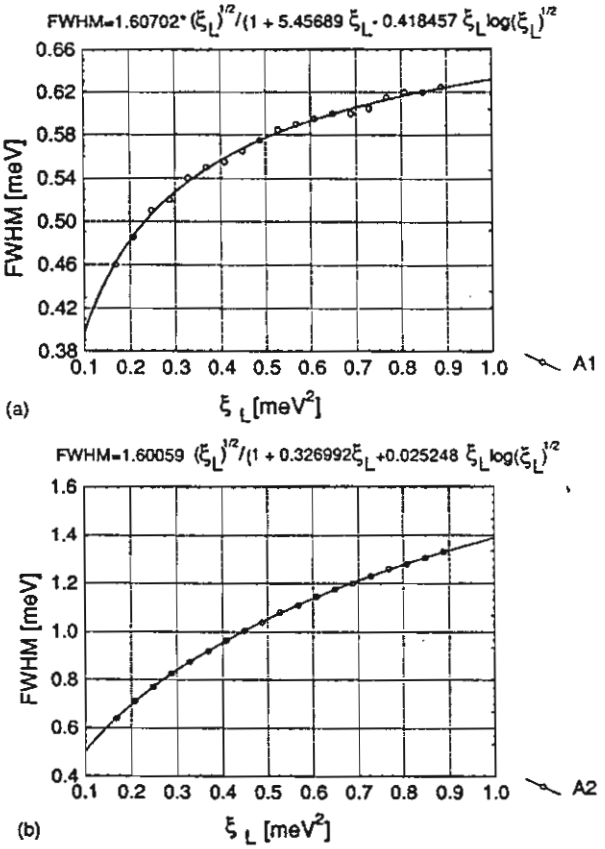

FIG. 8. Exciton absorption line width (FWHM) in meV vs variance of the random potential ξ_L for the first (a) and second cases (b) described in the text. The solid line represents a fit performed with the function derived by forcing the spectral density Eq. (32) to a Gaussian, taking the FWHM as the standard deviation (the exact values of the coefficients are shown at the top of the graph; $x=\xi_L$).

the spectrum is not a trivial one, as has been pointed out by Efros Wetzel,[2] but it has been shown to have an acceptable solution by Thouless and Elzain.[36] In order to determine the energy zero, we have calculated the energy-zero shift due to the disorder according to the expression [Eq. (9)] derived in the latter, which is

$$E_0^* = E_0 - \frac{w^2}{4\pi V}\left[1+\ln\left(\frac{128\pi V^2}{w^2}\right)\right], \tag{52}$$

where in the 2D case it has been shown[30,37] that the energy zero of the path-integral DOS occurs at $E_0=-4$ V. In calculating the energy-zero shift, we have taken into account the previously established relation between the disorder parameters introduced within the tight-binding model and the corresponding parameters in the path-integral approach,[30,37] namely, the tight-binding matrix element, representing the bandwidth $V=E_L$, and the variance $w^2=\xi_L$. The low-energy shift of the peak can be clearly seen, as well as the shift of the maximum to the left with increasing standard deviation (from $\sqrt{\xi_L}=0.41$ to 1 meV) of the random potential fluctuations.

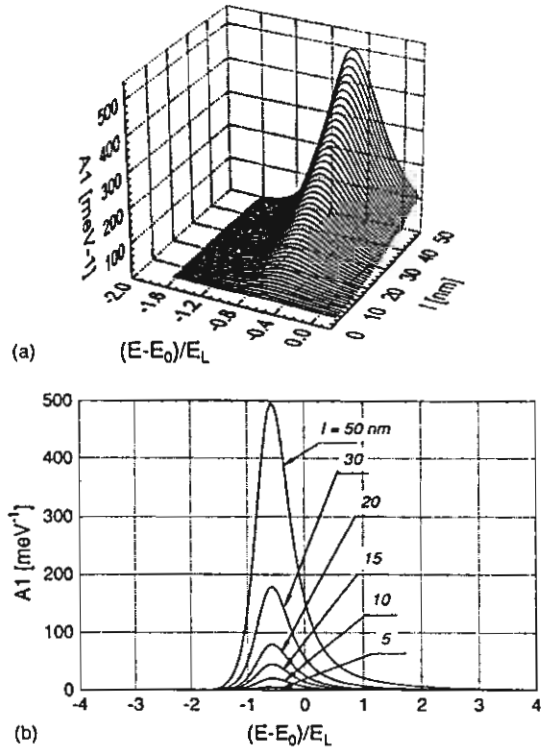

FIG. 9. (a) 3D plot of the optical density function corresponding to case 1 vs the energy, normalized with respect to the exciton correlation energy E_L and the correlation length l of the individual potentials. (b) Cross sections of (a): plots of the optical density function vs normalized energy corresponding to case 1 for $l=5,10,15,20,50$ nm.

The exciton linewidths calculated from these figures are $w=0.46$ and 0.62 meV for the first case and $w=0.63$ and 1.37 meV for the second case. In order to evaluate the asymmetry of the calculated spectra, it is convenient to define high- and low-energy linewidths w_{HE} and w_{LE}. The high-energy linewidths from Figs. 6(a) and 7(a) are 0.235 and 0.32 meV, while the low-energy linewidths are correspondingly 0.225 and 0.3 meV. Similarly, the high-energy linewidths inferred from Figs. 6(b) and 7(b) are 0.33 and 0.7 meV and the low-energy linewidths 0.3 and 0.67 meV. For both cases considered the high-energy linewidth is greater than the low-energy one, reflecting the steeper decay of the low-energy tail of the spectrum.

The exciton linewidths corresponding to the full path-integral derivation (case 2) seem to be in better agreement with the reported experimental widths than the ones with a high-energy tail calculated using the perturbation theory (case 1). We have compared the FWHM obtained at $\sqrt{\xi_L}=0.41$ meV (Fig. 6) with the exciton absorption linewidth of a single quantum well at $\sqrt{\xi_L}=0.4$ meV calculated in Ref. 5 (see Fig. 2). It should be noted that the second-case width of 0.63 meV is closer to the value $w=0.75$ meV obtained from Fig. 2 of Ref. 5. The observed agreement of the path-integral-inferred optical density spectra with the experimental data and up-to-date theoretical models can be attributed to the additional contribution of the localized exciton states

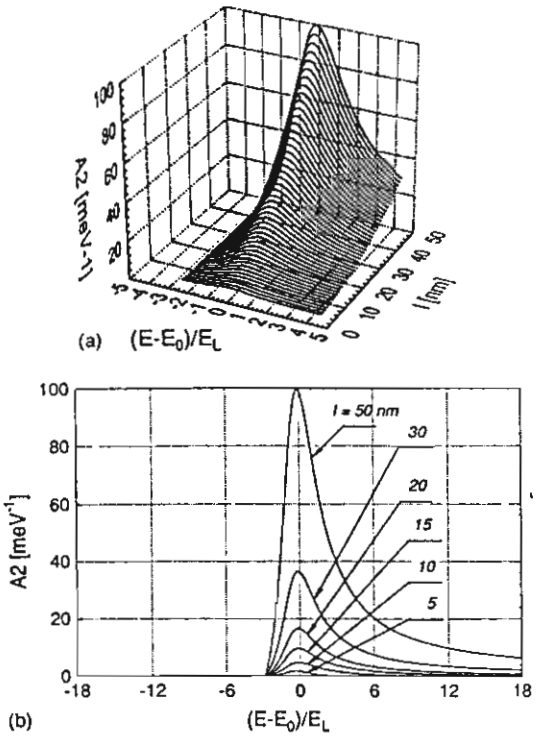

FIG. 10. (a) 3D plot of the optical density function corresponding to case 2 vs the energy, normalized with respect to the exciton correlation energy E_L and the correlation length l. (b) Cross sections of (a): plots of the optical density function vs normalized energy corresponding to case 2 for $l=5,10,15,20,50$ nm.

from the Kane band tail, while in the perturbation theory method only the contribution of the completely delocalized states is considered.

In Figs. 8(a) and 8(b) we have plotted the exciton absorption linewidth (FWHM) as a function of the variance of the random potential ξ_L, varying within the interval (0,1) for the first and second cases (the solid lines represent a fit to the data points). Both linewidths monotonically increase with increasing disorder and the relative broadening corresponding to the second case is greater than that for the first case. The best fit to the data is achieved using a function derived by forcing the spectral function from Eq. (32) to be Gaussian with standard deviation given by the FWHM. The FWHM in both cases depends to first order on the standard deviation $\sqrt{\xi_L}$ of the random potential, with higher-order terms giving rise to the asymmetric linewidth. Therefore instead of a normal (Gaussian) distribution of the spectral widths, characterized by a FWHM of $\sqrt{2\xi_L}$, we have obtained additional terms responsible for the asymmetric shape of the spectral function.

In our calculations (Sec. II) we introduced essentially two disorder parameters, namely, the variance of the random potential ξ_L and the correlation energy E_L. In order to study the effect of changing the correlation length of the potential fluctuations on the optical absorption spectrum we have fixed the variance at a value of $\sqrt{\xi_L}=0.5$ meV, varying only the correlation energy (or equivalently the correlation length). The interval of variation of the correlation lengths has been chosen in conformity with the value for the correlation energy $E_L=0.12$ meV of Zimmermann,[7] which gives $L \approx 9.61$ nm, i.e., L varies from 7 to 70 nm. The calculated optical density functions are presented in Figs. 9(a) and 9(b) and 10(a) and 10(b). In each figure represents a 3D plot (a) and (b) the corresponding 2D sections at different values of the correlation length; Figs. 9 and 10 are for the first and second cases under consideration, respectively. We have introduced the new variable l, according to $L=l\sqrt{2}$, where L is given in nanometers. It can be seen (Figs. 9 and 10) that increasing the correlation length (or equivalently l) and approaching the classical limit (i.e., $L\rightarrow\infty$ corresponding to perfect interface), the optical absorption spectrum tends to the free-exciton δ peak. In the opposite limit (decreasing the correlation length) continuous broadening of the exciton linewidth is observed, with a decrease in the peak magnitude and a low-energy shift of the maximum. In this case we approach the quantum case, which corresponds to the white-Gaussian-noise potential, when exciton localization takes place, resulting in the low-energy shift of the exciton peak. It should be noted, however, that these results are in contrast with the 2D optical absorption spectra calculated using linear optical susceptibility theory, shown in Fig. 6 of Ref. 18. where reduction of the correlation length reduces the FWHM and increases the magnitude of the peak.

To summarize, we believe that the classical limit of the optical density function can be reached in two equivalent ways, namely, either when the correlation length of the random potential fluctuations tends to infinity at a fixed depth of the potential fluctuations (as shown in Figs. 9 and 10) or by decreasing the magnitude (depth) of the potential fluctuations via ξ_L while keeping the correlation energy (or equivalently L) constant (as, e.g., in Fig. 5). In both cases we obtain as a limiting behavior at zero disorder the free-exciton δ peak of the optical absorption, since when the perturbation potential is switched off the exciton should move freely. Therefore we expect that on approaching the classical limit the exciton line shape will become more and more symmetric Lorentzian, which at zero disorder should reproduce the δ peak of free-exciton absorption. The opposite quantum limit is reached either when $L\rightarrow 0$, at a fixed depth ξ_L of the random potential fluctuations, or equivalently for energies deep in the excitonic band tail at a fixed correlation length L. In the first case the width of the typical potential well becomes increasingly smaller, while in the second case the potential well becomes deeper and steeper. Therefore increasing the disorder causes exciton localization to become more and more significant deep in the excitonic band tail, thus giving rise to Gaussian-Lorentzian-type asymmetric low-energy tails in the optical density.

IV. SUMMARY

In this paper we have developed a semianalytical quantum-mechanical description of the optical absorption spectrum for 2D excitons in a rough QW, taking into account exciton localization in the random potential fluctuations at the interface. The proposed method is based on the path-integral technique for calculating density of states in disordered systems. In this model the exciton c.m. motion near the interface in the field of the random individual scattering po-

tentials generated by local well-thickness fluctuations is considered. Gaussian statistics for the random distribution of the fluctuation potential is assumed. Asymptotic expressions for the low-and high-energy tails of the optical density function are obtained, and an alternative high-energy-tail asymptotic using the perturbation theory, limiting the absorption spectrum behavior at high energies and weak disorder, is also presented. Within the path-integral formalism two disorder parameters (characteristic energies) have been introduced, namely, the variance of the random potential fluctuations, representing a measure of the depth of the fluctuations, and the correlation energy, representing a measure of the exciton confinement. By using a nonlinear fitting procedure we have found an analytical interpolation function joining the two limiting asymptotics (for both cases under consideration) for any value of the variance of the random potential.

The calculated spectra exhibit the typical features observed in other methods of optical absorption calculations, such as the pronounced asymmetric shape, broadening of the excitonic line, and apparent low-energy shift of the maximum. Using the fitting parameters to the time-resolved experiments obtained in Ref. 7, a comparison has been made between the FWHM inferred from fully path-integral calculations and the calculations using perturbation theory for the high-energy tail. The comparison shows a much broader spectrum at strong enough disorder resulting from the fully path-integral approach than from the perturbation theory spectrum. This might be interpreted as due to the contribution of the localized exciton states in the high-energy tail of the spectrum, resulting from the semiclassical Kane tail in the density of states, which is absent within the perturbation theory approach, since only the free-exciton states are taken into account there. In both cases under consideration, we have found the leading term in the FWHM dependence on ξ_L to be proportional to the standard deviation of the random potential plus correction terms responsible for the asymmetric line shape.

We have also studied the effect of varying the correlation length of the random potential fluctuations on the optical density function. Our results are consistent in both classical and quantum limits, tending to the free-exciton peak at large correlation lengths and monotonically broadening in the quantum limit. The proposed method of calculation is relatively simple, since it uses analytical expressions for the optical density function across the whole energy range.

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Path integral derivation of Magnus force

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In this paper we derive the Magnus force from a model proposed by Ao and Thouless for treating the vortex tunneling in a superconductor with pinning potential and dissipation. We formulate this problem using the real time path integral and calculate the propagator exactly by first eliminating the x degree of freedom. The result is an effective action which renormalized the pinning potential as well as biasing the potential with the time dependence force which we identified as being the Magnus force. The fluctuation of the pinning potential is also discussed. [S0163-1829(99)04037-0]

In the past decade there has been an advance in material science which makes it possible to perform quantitative studies of the dynamic effect such as vortex dynamics, e.g., quantum creep[1] and anamolies in the Hall effect.[2] This effect plays an important role in the understanding of the mechanism of the existence of the Magnus force. The argument for the existence of a Magnus force was first proposed by Friedel, de Gennes, and Matricon[3] and later developed and extended by Nozieres and Vinen[4] by including pinning and friction. Although the Magnus force is believed to be a general property of the vortex line, the phenomenonological theory developed so far is still unsatisfactory.

The first microscopic theory that tries to explain the Magnus force is due to Ao and Thouless.[5] They derived the Magnus force by calculating the Berry phase for an adiabatic motion of the vortex. They also found that the existence of a Magnus force is a general property of the vortex line and is not influenced by the presence of the disorder and magnetic field. Since then there have been several attempts to derive the Magnus force from different fundamental approaches such as by the Chern-Simons Theory,[6] Feynman-Hellmann theorem,[7] etc.

The application of the Magnus force to tunneling in a quantized vortex again was given by Ao and Thouless.[8] In this work they considered the effect of the pinning potential in the two-dimensional xy plane and the dissipation of the vortex tunneling in a superconductor. They study this problem by using the imaginary time partition function path integral formalism. The Hamiltonian considered is

$$H=\frac{1}{2M}[\mathbf{p}-q_v\mathbf{A}(\mathbf{r})]^2+V(\mathbf{r}) +\sum_j\left[\frac{1}{2m_j}\mathbf{p}_j^2+\frac{1}{2}m_j\omega_j^2\left(\mathbf{q}_j-\frac{c_j}{m_j\omega_j^2}\mathbf{r}\right)^2\right], \quad (1)$$

where M is the vortex mass, $\mathbf{A}=h\rho_s d(y,0,0)/2$ is the vector potential, $d=$ the thickness of the film, $h=$ the Planck constant, $\rho_s=$ the superfluid electron number density, and the factor 1/2 comes from the Cooper pair, $q_v=+1(-1)$ standing for the parallelism (antiparallelism) in the $\hat{z}$ direction. The vortex pinning potential consists of two parts. The pinning potential in the x direction is approximated by a harmonic potential $(M/2)\Omega_x^2x^2$ and $V_y(y)$ is the pinning potential in the y direction which has a metastable state at $y=0$. The last term is the dissipative environment of the vortex consisting of a set of harmonic oscillators as formulated by Caldeira and Leggett.[9] The effect of the dissipative environment is specifed by the spectral function

$$J(\omega)=\pi\sum_j\frac{c_j^2}{2m_j\omega_j}\delta(\omega-\omega_j). \quad (2)$$

In this paper we derive the Magnus force from the real time propagator from the Feynman path integral instead of the imaginary time partition function path integral as discussed by Ao and Thouless. We believe that real time propagator gives direct information in interpreting the result.

Since we are interested in the derivation of the Magnus force, therefore we can neglect the dissipative environment. Their effect will be important for the tunneling problem and can be included if it is necessary. Then the model action becomes

$$S=\int_0^t d\tau\left[\frac{M}{2}\{\dot{\mathbf{r}}^2(\tau)+\omega\dot{x}(\tau)y(\tau)\} -\left\{V_y(y(\tau))+\frac{M}{2}\Omega_x^2x^2(\tau)\right\}\right], \quad (3)$$

where $\omega=\hbar\rho_s d$. Hence the propagator can be written as

$$K(y_2,y_1;x_2,x_1;t)=\int D[y(\tau)]D[x(\tau)]e^{(i/\hbar)S}. \quad (4)$$

To decouple this path integral, it is convenient to carry out partial integration in the second term of Eq. (3)

$$\int d\tau\dot{x}(\tau)y(\tau)=x_2y_2-x_1y_1-\int d\tau x(\tau)\dot{y}(\tau). \quad (5)$$

Then we can consider $\dot{y}$ as a generating functional or force oscillator of the propagator $K_x(x_2,x_1;t,\dot{y})$. The end points are not important and can be taken out from path integral. These end points are equivalent to the gauge transformation in the case of particle in the magnetic field. We thus get that

$$K(y_2,y_1;x_2,x_1;t)=\int D[y(\tau)]\exp\frac{i}{\hbar}\int_0^t d\tau\frac{M}{2}\{\dot{y}^2(\tau)-V_y[y(\tau)]\}K_x(x_2,x_1;t,\dot{y}), \quad (6)$$

where

$$K_x(x_2,x_1;t,\dot{y})=\int D[x(\tau)]\exp\frac{i}{\hbar}\int_0^t d\tau\times\left\{\frac{M}{2}[\dot{x}^2(\tau)-\Omega_x^2x^2(\tau)]+f(\tau)x(\tau)\right\}, \quad (7)$$

with $f(\tau)=M\omega\dot{y}(\tau)/2$. Carrying out the path integral in the x integration we obtain

$$K_x(x_2,x_1;t,\dot{y})=K_0(x_2,x_1;t)\exp\frac{i}{\hbar}\times\left\{\int_0^t d\tau\left[-F(\tau)y(\tau)-\frac{M\omega^2}{4}y^2(\tau)\right]+\int_0^t\int_0^t d\tau d\sigma y(\tau)y(\sigma)g(\tau,\sigma)\right\}, \quad (8)$$

where

$$K_0(x_2,x_1;t)=\left(\frac{M\Omega_x}{2\pi i\hbar\sin\Omega_xt}\right)^{1/2}\exp\left[\frac{i}{\hbar}\left(\frac{M\Omega_x}{2\sin\Omega_xt}\right)\times[\cos\Omega_x(t)(x_2^2+x_1^2)-2x_1x_2]\right]. \quad (9)$$

Here

$$F(\tau)=\frac{1}{2}\frac{M\omega\Omega_x}{\sin\Omega_xt}[x_2\cos\Omega_x\tau-x_1\cos\Omega_x(t-\tau)] \quad (10)$$

and

$$g(\tau,\sigma)=\frac{M\omega^2\Omega_x}{8\sin\Omega_xt}[\cos\Omega_x(t-\tau)\cos\Omega_x\sigma H(\tau-\sigma)+\cos\Omega_x(\tau-\sigma)\cos\Omega_x\tau H(\sigma-\tau)], \quad (11)$$

where $H(\tau-\sigma)$ is the Heaviside step function. In obtaining the above results we use the following identity:

$$\int_0^t\int_0^t d\tau d\sigma f(\tau)f(\sigma)G(\tau,\sigma)=\frac{M^2\omega^2}{4}\int_0^t\int_0^t d\tau d\sigma y(\tau)y(\sigma)\frac{d}{d\sigma}\frac{d}{d\tau}G(\tau,\sigma), \quad (12)$$

where

$$G(\tau,\sigma)=\frac{1}{2}[\sin\Omega_x(t-\tau)\sin\Omega_x\sigma H(\tau-\sigma)+\sin\Omega_x(t-\sigma)\sin\Omega_x\tau H(\sigma-\tau)]. \quad (13)$$

Differentiating $G(\tau,\sigma)$ twice we obtain

$$\frac{d}{d\sigma}\frac{d}{d\tau}G(\tau,\sigma)=-\frac{4\Omega_x\sin\Omega_xt}{M\omega^2}g(\tau,\sigma)+\Omega_x\sin\Omega_xt\,\delta(\tau-\sigma). \quad (14)$$

The second term of Eq. (14) gives the renormalized pinning potential in Eq. (8). Then the full propagator becomes

$$K(y_2,y_1;x_2,x_1;t)=K_0(x_2,x_1;t)\int D[y(\tau)]e^{(i/\hbar)S_{\rm eff}}, \quad (15)$$

where

$$S_{\rm eff}=\int_0^t d\tau\left[\frac{M}{2}\dot{y}^2(\tau)-\left\{V_y(y)+\frac{M}{4}\omega^2y^2(\tau)\right\}+F(\tau)y(\tau)\right]+\int_0^t\int_0^t d\tau d\sigma g(\tau,\sigma)y(\tau)y(\sigma). \quad (16)$$

Let us now discuss the physical meaning of each term in the $S_{\rm eff}$. The third term is a renormalization of the pinning potential in the y direction. The fourth term can be interpreted as the time dependent Magnus force and the last term represents the fluctuation due to the presence of the pinning potential in the x directon. To prove that $F(\tau)$ is the Magnus force, let us suppose that the weak pinning potential $\Omega_x\to 0$. Then $F(\tau)$ reduces to

$$F(\tau)=\frac{1}{2}M\omega\frac{x_2-x_1}{t}=\frac{1}{2}M\omega v_x$$

which is the Magnus force. This result is analogous to the Lorentz force and is also related to random systems as was pointed out by us in a previous paper.[10]

In conclusion we have demonstrated that by using the vortex model with pinning and dissipation, we can obtain the Magnus force by integrating out the x-degree of freedom. The resulting effective action is one-dimensional which contains several interesting results. First, the effective action renormalized the pinning potential $V_y(y)$ by $M\omega^2y^2(\tau)/2$ and secondly, it generated a linear driving force $F(\tau)$ which can be identified as the Magnus force. In order to proceed calculating further, it is necessary to know the pinning potential $V_y(y)$. Ao and Thouless[8] have proposed that the potential should be $V_y(y)=\hbar\rho_sd/2[-V_0y+\hbar|ny/2m_c|]$. This proposed potential consists of the pinning potential plus the image potential from the edge. Such a potential cannot be calculated analytically, therefore they did not discuss further their proposed potential. We note that, if one employs the saddle point potential i.e., $V_y(y)=-M\Omega_y^2y^2/2$, then the calculation can be done analytically. This problem is already discussed in our work concerning with the Landau level levitation in quantum Hall problems.[11] We further note that a recent paper by Kim and Shin[12] has considered the $V_y(y)$ as a cubic $V_y(y)=y^2-\alpha y^3$. In this case the analytical result

may be calculated exactly. Finally we mention the fluctuation contribution in Eq. (16) which arises from the fluctuation of the Ω_x effect on the y coordinate. If we add the dissipation contribution from the environment, then this fluctuation combines with the environmental contribution to give the so call anomalous damping kernel in the Ao and Thouless works.[8]

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Magnus force and Hellmann–Feynman force: path integral approach

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Abstract

This paper considers the derivation of the Magnus force from a model system consisting of a single vortex imbedded in a uniform positive background coupled with a mutual interaction charged boson. By eliminating the charged boson degree of freedom, the effective action of a single vortex is obtained and can be used to derive the Hellmann–Feynman force. From the ground state contribution a Magnus force is obtained.

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The Magnus force or lift force of classical hydrodynamics arises as a consequence of its motion through the fluid. The argument for the existence of a Magnus force on a vortex line in the type II superconductor was first proposed by Friedel *et al* [1] and later developed and extended by Nozieres and Vinen [2] by including pinning and friction. It was believed that the existence of a vortex is a general property of the system. In this paper we show that the existence of the Magnus force is a general property of a vortex. We propose a microscopic derivation of the Magnus force from a model system consisting of a single vortex coupled to mutual-interacting charged bosons and imbedded in a uniform positive background. By eliminating the charged boson degree of freedom an effective Lagrangian is obtained containing the generalized Hellmann–Feynman force which can be used to derive the Magnus force. This force can be obtained by considering that the ground state contribution leads to the Magnus force.

The full Hamiltonian for a quantized vortex coupled to an interacting charged boson imbedded in a positive uniform background is given as

$$\hat{H} = \hat{H}_v + \hat{h}_c + \hat{h}. \tag{1}$$

Here, $H_v(\hat{\vec{P}}, \hat{\vec{R}})$ is the Hamitonian for a quantized vortex in which $\vec{R}$ denotes the position of the vortex and $\vec{P}$ its conjugate momentum. The second term

$$\hat{h}_c = -\frac{e^2}{2m^2c} \sum_{n \neq n'} p_n^i T^{ij}(\vec{x}_n - \vec{x}_{n'}) p_{n'}^j \tag{2}$$

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with $T^{ij}(\vec{x}) = (\delta^{ij}|\vec{x}|^{-1} + x^i x^j|\vec{x}|^{-3})/2c$, the current–current interaction, and m is the boson mass. The Hamiltonian $\hat{h}_c$ represents the lowest-order relativistic effects, an interaction first obtained by Darwin in 1920 [3]. The last term

$$\hat{h} = \sum_n \frac{\left(\hat{\vec{p}}_n - \frac{2e}{c}\hat{\vec{a}}(\hat{\vec{x}}_n - \hat{\vec{R}})\right)^2}{2m} + \frac{1}{2}\sum_{n\neq n'} U(\hat{\vec{x}}_n - \hat{\vec{x}}_{n'}) + \hat{h}_b \tag{3}$$

is the Hamiltonian representing N bosons with negative charge $-e$, interacting with the vector potential $\vec{a}(\hat{\vec{x}}_n - \hat{\vec{R}})$ and satisfying the equation $\oint \vec{a}(\vec{x}_n - \vec{R})\cdot d\vec{l} = \phi_0 = hc/2e$. The $U(\hat{\vec{x}}_n - \hat{\vec{x}}_{n'})$ term represents the mutual Coulomb interaction. Finally $\hat{h}_b$ is the uniform positive background and

$$\hat{h}_b = -\sum_n \int d^3\vec{x}' e^2 \bar{n}(\vec{x}')|\vec{x}_n - \vec{x}'|^{-1} \tag{4}$$

where $\bar{n}(\vec{x}')$ is the charge distribution of the lattice and accounts for the interaction with the uniform positive background charge $e\bar{n}$.

Next, the full Hamiltonian $\hat{H}$ can be separated into two parts—the internal and the collective. The internal part, $\hat{h}_i = \hat{h} + \hat{h}_c$, is dependent on the centre point of the vortex, $\vec{R}$, and not explicitly on the conjugate momentum of the vortex, $\vec{P}$. The collective Hamiltonian, $\hat{H}_v$, is the Hamiltonian for a quantized vortex.

In considering the probability amplitude for a quantum process starting from the initial position, $\vec{x}_{a1}, \ldots, \vec{x}_{aN}, \vec{R}_a$ at t_a, and returning to the final position $\vec{x}_{b1}, \ldots, \vec{x}_{bN}, \vec{R}_b$ at t_b, the propagator can be written as

$$K(\vec{x}_{1b}, \ldots, \vec{x}_{Nb}, \vec{R}_b, t_b; \vec{x}_{1a}, \ldots, \vec{x}_{Na}, \vec{R}_a, t_a) = \sum_m \sum_n \Psi_m(\vec{x}_{1b}, \ldots, \vec{x}_{Nb}; \vec{R}_b)$$
$$\times \langle m; \vec{R}_b|\langle \vec{R}_b| \exp\left[-\frac{i}{\hbar}\hat{H}(t_b - t_a)\right]|\vec{R}_a\rangle|n; \vec{R}_a\rangle \Psi_n^*(\vec{x}_{1a}, \ldots, \vec{x}_{Na}; \vec{R}_a). \tag{5}$$

By inserting complete sets of coordinate states and a complete set of momentum states at $t = t_k$, with $\varepsilon = \frac{t_b - t_a}{L}$ it is possible to consider the following relationship as $\varepsilon \to 0$

$$\langle \vec{R}_k| \exp\left[-\frac{i}{\hbar}\hat{H}\varepsilon\right]|\vec{R}_{k-1}\rangle \approx \langle \vec{R}_k| \exp\left[-\frac{i}{\hbar}\hat{\vec{H}}_v(\hat{\vec{P}}, \hat{\vec{R}})\varepsilon\right]|\vec{R}_{k-1}\rangle \exp\left[\frac{i}{\hbar}\hat{h}_i(\hat{\vec{x}}, \hat{\vec{p}}; \vec{R}_k)\varepsilon\right]$$
$$= \int d\vec{P}_k \exp\left[\frac{i}{\hbar}\varepsilon\left[\vec{P}_k \cdot \left(\frac{\vec{R}_k - \vec{R}_{k-1}}{\varepsilon}\right) - \hat{H}_v(\hat{\vec{P}}, \hat{\vec{R}})\right]\right] \exp\left[\frac{i}{\hbar}\hat{h}_i(\hat{\vec{x}}, \hat{\vec{p}}; \vec{R}_k)\varepsilon\right]. \tag{6}$$

Then equation (5) can be expressed as

$$K(\vec{x}_{1b}, \ldots, \vec{x}_{Nb}, \vec{R}_b, t_b; \vec{x}_{1a}, \ldots, \vec{x}_{Na}, \vec{R}_a, t_a)$$
$$= \sum_m \sum_n \Psi_m(\vec{x}_{1b}, \ldots, \vec{x}_{Nb}; \vec{R}_b)\Psi_n^*(\vec{x}_{1a}, \ldots, \vec{x}_{Na}; \vec{R}_a)$$
$$\times \int D[\vec{P}]D[\vec{R}]T_{mn} \exp\left[-\frac{i}{\hbar}S[\vec{R}(t), \vec{P}(t)]\right] \tag{7}$$

where $S[\vec{R}(t), \vec{P}(t)] = \int_{t_a}^{t_b}[\vec{P}\cdot\dot{\vec{R}} - H_v(\vec{P}, \vec{R})]dt$ is the action of the collective motion along the path between a and b. Here, $\Psi_n(\vec{x}_{1a}, \ldots, \vec{x}_{Na}; \vec{R}_a)(\Psi_m(\vec{x}_{1b}, \ldots, \vec{x}_{Nb}; \vec{R}_b))$ are the wavefunctions of the internal part, $\hat{h}_i = \hat{h} + \hat{h}_c$ at $\vec{R} = \vec{R}_a(\vec{R}_b)$ with eigenvalue $E_n(\vec{R}_a)(E_m(\vec{R}_b))$ and the external variable $\vec{R} = \vec{R}_a(\vec{R}_b)$. T_{mn} is just the transition amplitude

between the quantum states from $\Psi_m(\vec{x}_{1b}, \ldots, \vec{x}_{Nb}; \vec{R}_b)$ to $\Psi_n(\vec{x}_{1a}, \ldots, \vec{x}_{Na}; \vec{R}_a)$ and is given by

$$T_{mn} = \langle m; \vec{R}_b | \exp\left[-\frac{\mathrm{i}}{\hbar}\hat{h}_i(\vec{R}(t_b))\varepsilon\right] \cdots \exp\left[-\frac{\mathrm{i}}{\hbar}\hat{h}_i(\vec{R}(t_a))\varepsilon\right] | n; \vec{R}_a\rangle. \tag{8}$$

By inserting the completeness relationship holding for the internal state $\hat{h}_i$ at each point of the external variable $\vec{R}_k$, $\sum_{j_k} |j_k; \vec{R}_k\rangle\langle j_k; \vec{R}_k| = 1$, equation (8) can be written as

$$T_{mn} = \sum_{j_1} \cdots \sum_{j_L} \langle m; \vec{R}_b | \exp\left[-\frac{\mathrm{i}}{\hbar}\hat{h}_i(\vec{R}(t_b))\varepsilon\right] | j_L; \vec{R}_L\rangle \cdots$$
$$\times \langle j_1; \vec{R}_1 | \exp\left[-\frac{\mathrm{i}}{\hbar}\hat{h}_i(\vec{R}(t_a))\varepsilon\right] | n; \vec{R}_a\rangle. \tag{9}$$

In the adiabatic approximation, an example is Berry's 1985 phase [4], the quantum transition between states with the same quantum number n only is picked up and is described by the matrix element $\langle n; \vec{R}_{k+1} | \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{h}_i(\vec{R}_i)\varepsilon} | n; \vec{R}_k\rangle$. Thus by using the approximate relation

$$\langle n; \vec{R}_{k+1} | \exp\left[\frac{\mathrm{i}}{\hbar}\hat{h}_i(\vec{R}_k)\varepsilon\right] | n; \vec{R}_k\rangle \approx [1 - \langle n; \vec{R}|\vec{\nabla}_R|n; \vec{R}\rangle \cdot \dot{\vec{R}}\varepsilon] \exp\left[-\frac{\mathrm{i}}{\hbar}\varepsilon E_n(\vec{R}_k)\right]$$
$$= \exp\left[\frac{\mathrm{i}}{\hbar}\varepsilon(-E_n(\vec{R}_k) + \mathrm{i}\hbar\vec{A}_{n,n} \cdot \dot{\vec{R}})\right] \tag{10}$$

equation (8) becomes

$$T_{mn} = \delta_{m,n} \exp\left[-\frac{\mathrm{i}}{\hbar}\int_{t_a}^{t_b} (E_n(\vec{R}) - \mathrm{i}\hbar\vec{A}_{n,n} \cdot \dot{\vec{R}})\mathrm{d}t\right] \tag{11}$$

where

$$\vec{A}_{n,n} = \langle n; \vec{R}|\vec{\nabla}_R|n; \vec{R}\rangle. \tag{12}$$

The vector potenial $\vec{A}_{n,n}$ implies the property of the internal part of the Hamiltonian $\hat{h}_i$ in the form of ket vector $|n; \vec{R}\rangle$. We arrive at the effective path integral associated with the adiabatic approximation of the dynamical variable $\vec{R}$,

$$K(\vec{x}_{1b}, \ldots, \vec{x}_{Nb}, \vec{R}_b, t_b; \vec{x}_{1a}, \ldots, \vec{x}_{Na}, \vec{R}_a, t_a)$$
$$= \sum_m \sum_n \Psi_m(\vec{x}_{1b}, \ldots, \vec{x}_{Nb}; \vec{R}_b)\Psi_n^*(\vec{x}_{1a}, \ldots, \vec{x}_{Na}; \vec{R}_a)K_{mn} \tag{13}$$

K_{mn} gives the usual dynamical evolution of the wavefunction of the internal part with an additional effect from the motion of the external variable over all possible paths. Therefore, the evolution kernel K_{mn} can be expressed as,

$$K_{mn} = \delta_{m,n}\int D[\vec{P}]D[\vec{R}]\exp\left[\frac{\mathrm{i}}{\hbar}\left[\int_{t_a}^{t_b}\mathrm{d}t([\vec{P} \cdot \dot{\vec{R}} - H_v] - E_m(\vec{R}) + \mathrm{i}\hbar\vec{A}_{n,n} \cdot \dot{\vec{R}})\right]\right] \tag{14}$$

where, $L_{n,n}^{\mathrm{eff}} = [\vec{P} \cdot \dot{\vec{R}} - H_v] - E_n(\vec{R}) + \mathrm{i}\hbar\vec{A}_{n,n} \cdot \dot{\vec{R}}$ is the effective Lagrangian corresponding with Schrödinger's equation for molecular physics given by the Born–Oppenheimer approximation [5], a matrix-valued Schrödinger operator for the nuclear wavefunction. If the external variable $\vec{R}(t)$ is to describe an adiabatic motion returning via a closed path C then the third term in the exponent of equation (14) is immediately recognized as Berry's 1985 phase [4]:

$$\Gamma_n = \mathrm{i}\hbar\oint_C \langle n; \vec{R}|\vec{\nabla}_R|n; \vec{R}\rangle \cdot \mathrm{d}\vec{R}. \tag{15}$$

To obtain the Hellmann–Feynman force, we define the force on the vortex from the Lagrange equation

$$\frac{\partial}{\partial \vec{R}}L_m^{\mathrm{eff}} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial}{\partial \dot{\vec{R}}}L_m^{\mathrm{eff}} = 0. \tag{16}$$

Then the new force, which is in addition to the original force, can be written as

$$F_m^X = i\hbar \dot{R}^X \left[\left\langle \frac{\partial \Psi_m}{\partial Y} | \frac{\partial \Psi_m}{\partial X} \right\rangle - \left\langle \frac{\partial \Psi_m}{\partial X} | \frac{\partial \Psi_m}{\partial Y} \right\rangle \right] - \frac{\partial}{\partial X} E_m(\vec{R}) \tag{17}$$

$$F_m^Y = i\hbar \dot{R}^Y \left[\left\langle \frac{\partial \Psi_m}{\partial Y} | \frac{\partial \Psi_m}{\partial X} \right\rangle - \left\langle \frac{\partial \Psi_m}{\partial X} | \frac{\partial \Psi_m}{\partial Y} \right\rangle \right] - \frac{\partial}{\partial Y} E_m(\vec{R}). \tag{18}$$

The above result can be easily recognized as the Hellmann–Feynmen theorem [6]. Next the Magnus force can be derived by using the many-body wavefunction proposed by Ao and Thouless [7]. This wavefunction contains both amplitude and phase varying in space and time

$$\Psi_0(\vec{x}_1, \ldots, \vec{x}_N; \vec{R}) = \tilde{\Psi}_0(\vec{x}_1, \ldots, \vec{x}_N; \vec{R}) \exp\left[\frac{i}{\hbar} \sum_{j=1}^{N} \Theta(\vec{x}_j - \vec{R}) \right] \tag{19}$$

where $\tilde{\Psi}_0$, in the absence of the external magnetic field, is the many-body wavefunction of a superconductor. The ground state wavefunction depends on the positions of the N bosons in the system. Since the wavefunction can be determined in such a way that the dependence on $\vec{x}$ is entirely through $\vec{x} - \vec{R}$, the partial derivatives with respect to $\vec{R}$ can be replaced by a sum over partial derivatives with respect to the particle coordinate $\vec{x}_i$. The probability of any particular configuration is proportional to $|\tilde{\Psi}_0|^2$, with the normalization,

$$\int \cdots \int |\tilde{\Psi}_0|^2 d^2\vec{x}_1 \cdots d^2\vec{x}_N = N \tag{20}$$

and

$$\int \cdots \int |\tilde{\Psi}_0|^2 d^2\vec{x}_1 \cdots d^2\vec{x}_{N-1} = \rho(\vec{x}, \vec{R}) \tag{21}$$

where $\rho(\vec{x}, \vec{R})$ is the probability density. The probability density $\rho(\vec{x}, \vec{R})$ must satisfy the boundary conditions; that is, the density $\rho(\vec{x}, \vec{R})$ must vanish continuously at $\vec{x} = \vec{R}$ as well as approach the background density ρ_0 as $|\vec{x} - \vec{R}| \to \infty$. Therefore, the Magnus force from the first term in equations (17) and (18) can be defined as,

$$\vec{F}_{\text{Magnus}} = \dot{\vec{R}} \times i\hbar \vec{\nabla}_R \times \langle \Psi_0; \vec{R} | \vec{\nabla}_R | \Psi_0; \vec{R} \rangle. \tag{22}$$

By virtue of the property of the many-body wavefunction and the ground state condition, the Magnus force becomes

$$\vec{F}_{\text{Magnus}} = \dot{\vec{R}} \times \vec{\nabla}_R \times \int d^2\vec{x} N \rho(\vec{x}, \vec{R}) \vec{\nabla}_R \Theta(\vec{x} - \vec{R}). \tag{23}$$

Using Stokes theorem and the relation

$$\vec{\nabla}_R \Theta(\vec{x} - \vec{R}) = \frac{\hat{k} \times (\vec{x} - \vec{R})}{|\vec{x} - \vec{R}|^2} \tag{24}$$

the following equation is finally obtained:

$$\vec{F}_{\text{Magnus}} = 2\pi \rho_s \hbar \hat{k} \times \dot{\vec{R}} \tag{25}$$

where $\rho_s = N\rho_0$ is the number density.

Thus, a force is exerted on the vortex when it moves relative to the fluid density. This Magnus force is proportional to and perpendicular to the vortex velocity, and proportional to the fluid density. The Magnus force makes the vortex dynamics similar to that of charged particles in a magnetic field, with the role of the magnetic field played by the fluid density. This problem is discussed in our previous papers [8, 9]. However, it is interesting to point out that in this formulation, the mass of the vortex in the canonical momentum $\vec{P}$ was deliberately

hidden. The mass of the vortex is still controversial; this is addressed in another paper [10]. In conclusion we have demonstrated that the origin of the Magnus force is an effect of the transition amplitude of the supercurrent and is independent of the mutual interaction of the boson. The quantum transition between states is a result of interaction between the vector potenial of a vortex and a supercurrent or charged boson. The existence of the Magnus force in a neutral fluid is an effect of pressure. This is the difference between the Magnus force in a superconductor and that in a neutral fluid. These findings support the belief that the Magnus force is a general property of the system.

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Path Integral Derivation of the Effective Mass of Vortex

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Abstract

In this paper we derive the mass of the vortex from the effective Lagrangian proposed by Ao and Thouless[1] which contain the magnus force and dissipation terms. By using the Feynman-Jensen variational principle we obtain the dynamic and cyclotron mass of the vortex. We also discussed the finiteness of the dynamic mass.

Introduction

Vortex plays an important role in understanding of both the dynamic and static properties of superfluidity. The theoretical understanding of the vortex is based on the phenomenological approach. The idea is to write down the equation of vortex involving the effective mass, the magnus force and the friction. Since the vortex mass play an important role in the tunnelling process, therefore it is sensible to consider the effective mass derived from the microscopic theory. There have been several attemps to derive the effective mass of vortex from the classical theory. The earlier attempts to estimate the effective mass was given by Duan[1] via using the classical equations. Similar approach was also considered by Sin[2]. He showed that the significant contribution to the inertial mass of the vortex in a superconductor may come from lattice deformation of the vortex core.

Duan also considered the effective mass by using the concept of infinite compressibility of the fluids to consider the problem of inertial mass of the vortex line in both neutral and charged superfluids near zero temperature. By using the time-dependent Ginzburg-Landau theory he showed that the inertial masses diverge logarithmically with the sample for the neutral superfluids.

The first microscopic description of the effective mass was due to Ao[3] by using the Feynman many-body wave function for superfluid film containing vortex they shown that the vortex effective mass cannot be infinite. They also showed that in the case of super Ohmic damping, the spectral function $J(\omega)$ varies as ω^2 at low frequencies, the effective mass becomes logarithmically divergent. Since the problem of the vortex inertial mass in superfluids is a complicated issue, there are no clear calculations of the effective mass. The theoretical estimation of the effective mass of the vortex range from zero [2] to finite [3] and to infinite [4].

It is interesting to mention the recent work on calculation of the effective mass of the vortex [5] using the effective action within non-local in time term. They derive the mass formula and compute the integral of the spectral function

$\frac{J(\omega)}{\omega^3}$ over various frequencies. The results confirm their previous work using the Feynman wave function approach.

In this paper we derive the effective mass from the microscopic model given by Ao and Thouless[1] and demonstrate that by using the density matrix in the path integral formula developed by us in the previous paper for handling the polaron effective mass (Sa-yakanit[6]). We will show in this paper that for zero temperature limit and short distance, the density matrix reads as

$$\rho(\vec{x_2} - \vec{x_1}, \beta) \approx e^{-E_o\beta - \frac{m_d}{2\beta}|\vec{x_2}-\vec{x_1}|^2 + \frac{m_c\omega}{2}(x_2y_1 - x_1y_2)} \tag{1}$$

where E_o is the ground state energy of the system and β denotes the imaginary time. One can see from this expression that there appear two types of mass i.e. the dynamic type and the cyclotron type. It was also pointed out by Unk[7] that in this case, the dynamic mass goes to infinity. Hence the definition of the cyclotron effective mass is more appropriate. We can show the logarithmic divergence of the mass is a consequence of the super Ohmic assumption, $J(\omega) \sim \omega^3$. For analytical calculations we assume that the spectral is $J(\omega) = \omega^s e^{-\omega}$, where s is a real number and ω_c is the cutoff frequency.

Our starting point is the model Lagrangian given by

$$H = \frac{1}{2m}[\mathrm{p} - q_v\mathrm{A}(\mathrm{r})]^2 + V(\mathrm{r}) + \sum_j [\frac{1}{2m_j}\mathrm{p}_j^2 + \frac{1}{2}m_j\omega_j^2(\mathrm{q}_j - \frac{c_j}{m_j\omega_j^2}\mathrm{r})^2] \tag{2}$$

where $\mathrm{A} = \frac{1}{2}h\rho_s d(\eta, 0, 0)$ and $\nabla \times \mathrm{A} = h\rho_s d\dot{x}y$

Integrating out the degree of freedom $\{\mathrm{q}_j\}$ we have the effective action

$$\begin{aligned} S_{eff} &= \int_0^\beta dt[\frac{m}{2}\dot{\mathrm{r}}^2 + \frac{1}{2}i\eta q_v\rho_s d\dot{x}y] \\ &+ \int_0^\beta dt \int_0^\beta ds K(t-s)|\mathrm{r}(t) - \mathrm{r}(s)|^2. \end{aligned} \tag{3}$$

where $K(t-s) = \frac{1}{\pi}\int_0^\infty d\omega J(\omega)\frac{\cosh[\omega(\frac{\beta}{2} - |t-s|)]}{\sinh(\frac{\omega\beta}{2})}$ and $J(\omega) = \pi\sum_j \frac{c_j^2}{2m_j\omega_j}\delta(\omega - \omega_j)$

In this paper we model the model system by a quadratic trial action

$$S_o = \int_0^\beta dt\frac{m}{2}\dot{\mathrm{r}}^2 - \frac{C}{4}\int_0^\beta dt\int_0^\beta ds|\mathrm{r}(t) - \mathrm{r}(s)|^2\frac{\cosh[\Omega(\frac{\beta}{2} - |t-s|)]}{\sinh(\frac{\Omega\beta}{2})} \tag{4}$$

where C and ω are two parameters to be determined. Physically, we model the whole system by the system of a vortex attached to a fictitious particle of mass M with spring constant κ [6]. The justification of modelling both the magnus

force and the dissipation is that the magnus force can be rewritten in terms of a non-local action as discussed in our previous paper [7].

In order to obtain the effective mass of the vortex we consider the imaginary time density matrix of the system as

$$\rho(\vec{x_2},\vec{x_1},\beta) = \int_{x_1}^{x_2} D[x]e^{-S_{eff}} \tag{5}$$

With the first cumulant expansion we have

$$\rho(\vec{x_2},\vec{x_1},\beta) \approx \rho_0 e^{-\langle S_{eff}-S_0\rangle_{S_0}} \tag{6}$$

where $\langle O\rangle_{S_0} = \frac{\int D[x]Oe^{-S_0}}{\int D[x]e^{-S_0}}$

Following the scheme of the Feynman polaron [8] and our pervious work [6], the density matrix becomes

$$\begin{aligned}\rho &= \rho_0 \exp -\{\int_0^\beta\int_0^\beta dtds[\int_0^\infty d\omega\frac{J(\omega)}{\pi}\frac{\cosh\omega(\frac{\beta}{2}-|t-s|)}{\sinh(\frac{\omega\beta}{2})} \\ &\quad -\frac{C}{2}\frac{\cosh\Omega(\frac{\beta}{2}-|t-s|)}{\sinh(\frac{\Omega\beta}{2})}]\chi + \frac{i\rho qd}{2}\int_0^\beta dt[x_2\Phi+x_1\Psi] \\ &\quad \times[y_2\frac{d\Phi}{dt}+y_1\frac{d\Psi}{dt}]\}\end{aligned} \tag{7}$$

where

$$\rho_0 = (\frac{m}{2\pi\beta})(\frac{v}{\Omega}\frac{\sinh(\frac{\Omega\beta}{2})}{\sinh(\frac{\nu\beta}{2})})^2 exp-[\frac{\mu\nu}{4}\coth(\frac{\nu\beta}{2})+\frac{\mu}{2M\beta}](\mathrm{r}_2-\mathrm{r}_1)^2 \tag{8}$$

with

$$\begin{aligned}\chi &= \frac{2\mu}{m}(\frac{2\sinh\frac{\nu\beta}{2}(t-s)\sinh\frac{\nu}{2}(\beta-|t-s|)}{m\nu\sinh(\frac{\nu\beta}{2})}+\frac{(\beta-|t-s|)(t-s)}{M\beta}) \\ &\quad +\mu^2(\frac{\sinh\frac{\nu\beta}{2}(t-s)\cosh\frac{\nu}{2}(\frac{\beta}{2}-(t+s))}{m\sinh(\frac{\nu\beta}{2})}+\frac{(t-s)^2}{M\beta})[\mathrm{r}_2-\mathrm{r}_1]^2 \\ \Phi &= \frac{\mu}{m}[\frac{\sinh(\nu t)}{\sinh(\nu\beta)}+\frac{\sinh\frac{\nu}{2}(\beta-t)\sinh\frac{\nu t}{2}}{\cosh(\frac{\nu\beta}{2})}]+\frac{\mu t}{M\beta} \\ \Psi &= \frac{\mu}{m}[\frac{\sinh\nu(\beta-t)}{\sinh(\nu\beta)}+\frac{\sinh\frac{\nu}{2}(\beta-t)\sinh\frac{\nu t}{2}}{\cosh(\frac{\nu\beta}{2})}]+\frac{\mu(\beta-t)}{M\beta}\end{aligned}$$

and the parameters are defined by

$$C=\frac{M\Omega^3}{4}, \Omega^2=\frac{\kappa}{M}, \nu^2=\frac{\kappa}{\mu}, \mu=\frac{mM}{m+M}, \mathrm{r}=(x,y). \tag{9}$$

Among these four parameters we can choose any two independent variational parameters. In order to obtain the effective mass, we take the limit as

$\beta \to \infty$ and $(\vec{x_2} - \vec{x_1}) \to 0$. Then up to the first order correction term, we have

$$\rho(\vec{x_2} - \vec{x_1}, \beta \to \infty) \approx \exp(-E_o\beta - \frac{m_d}{2\beta}|\vec{x_2} - \vec{x_1}|^2 + \frac{m_c\omega}{2}(x_2y_1 - x_1y_2)) \quad (10)$$

We can derive the ground state energy E_o from the diagonal part of the density matrix by direct integration of the exponent together with the contribution from ρ_o and then obtain

$$\begin{aligned} E_o &= \frac{(\nu - \Omega)^2}{2\nu} + \frac{2\mu}{\pi m}\int_0^\infty d\omega J(\omega)[\coth(\frac{\omega\beta}{2})(\frac{1}{m(\omega^2 - \nu^2)} + \frac{1}{M\omega^2}) \\ &\quad - \frac{\nu}{m\omega(\omega^2 - \nu^2)}\coth(\frac{\nu\beta}{2})] \end{aligned} \quad (11)$$

When $\beta \to \infty$ and by using the relations in equation(9) we can approximate the ground state energy as

$$E_o = \frac{\nu}{2}(1 - \sqrt{\frac{M}{1+M}})^2 + \frac{2\mu}{\pi}\int_0^\infty d\omega J(\omega)(\frac{1}{\omega(\omega+\nu)} + \frac{1}{\omega^2 M}) \quad (12)$$

where the bare mass m was set to unity for simplicity. To derive the dynamics mass which concerns translational invariant terms in the exponent of the density matrix, we follow the scheme in the reference[6] which the coordinates were transformed to the center of mass system $(\vec{r_2} - \vec{r_1}) \to (\frac{m+M}{m})(\vec{R_2} - \vec{R_1})$. Then the effective dynamic mass of the vortex is

$$m_d = m + \frac{4}{\pi}\int_0^\infty d\omega \frac{J(\omega)}{\omega^3} \quad (13)$$

Note that this effective masss is independent of the variational parameters. Now we consider the part arising from the magnus force. We interpret the mass emerge in front of the terms $(x_2y_1 - x_1y_2)$ as the effective cyclotron mass since it make the vortex move in the manner analogous to a charged particle in a magnetic field. Hence the terms in the exponent are :

$$m_c = \frac{\rho q d}{\omega_c}(\frac{\mu}{2m})^2\int_0^\beta dt[\nu e^{-\nu t} + \frac{2m}{M\beta}][(1 + e^{-\nu t}) + \frac{2m}{M} - \frac{2mt}{M\beta}] \quad (14)$$

We now can discuss our results. As we can see from equations (13) and (14), the effective mass arises from both the magnus force term and the dissipation of the system as the integral of the spectral function $\frac{J(\omega)}{\omega^3}$. This expression suggests that for finite mass, the spectral function must proper to ω^3 which is the super Ohmic case. For $J(\omega) \sim \omega^2$, the result becomes the logarithmic diverge as discussed

earlier by Duan[4] and Ao[1]. It is worth mentioning that the term $\frac{J(\omega)}{\omega^3}$ has also been obtained recently by Han, Ao and Zhu[5] having the effective action without the magnus force. In case of the effective mass diverge, it is more appropriate to discuss the cyclotron mass. Physically, the diverge dynamic effective mass corresponds to the vortex cannot move therefore the cycloton mass is more appropriate. In order to get into more detailed calculation we determine the two variational parameters C and Ω by minimizing the ground state energy with respect to these parameters and we obtain the upper bound of the ground state energy according to the Feynman-Jensen Inequality. As pointed out by Feynman, since there is no variational principle for the excited states the parameters obtained from minimizing the ground state are used to determine the effective mass. This was demonstrated in the polaron problem[12]. We also employ this method to obtain the two parameters.

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Localization and the Effective Mass of a Vortex

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Abstract

In the problem of a vortex escaping from a metastable potential, we derive the localization criterion of a vortex at finite dissipation and temperature by analyzing both the crossover temperature formula and the escape rate formula. In the absence of a pinning potential in the stable direction, this criterion shows that a vortex will be localized in a metastable potential when the Magnus force is strong enough. Using the concept of this localization criterion, the effective mass of a vortex can be defined and interpreted. Moreover, the role of pinning and dissipation in the process of vortex escape can also be discussed.

In this paper, we present an analytical study on vortex escaping in the presence of the Magnus force, pinning, and dissipation. This study leads to many condusions concerning the roles of pinning and dissipation and especially the localization and the effective mass of a vortex.

We start with the Hamiltonian for a vortex moving in a two dimensional x-y plane, which can be regarded as a point particle, in the form[1]

$$H = \frac{1}{2M}|\vec{P} - q_\nu \vec{A}(\vec{r})|^2 + \sum_j [\frac{1}{2m_j}|\vec{P}_j|^2 + \frac{1}{2}m_j\omega_j^2|\vec{q}_j - \frac{c_j}{m_j\omega_j^2}\vec{r}|^2], \qquad (1)$$

with the vector potential $\vec{A}$ determined by $\vec{\nabla}\times\vec{A} = (M\Omega/q_\nu)\hat{z}$. Here $q_\nu = +1(-1)$ stands for the vorticity paralleling (antiparalleling) to the unit vector $\hat{z}$ in the z direction, M is the vortex mass, and Ω is the frequency dimensional parameter which is equal to $q_\nu h\rho_s d/2M$ for a vortex in superconductor (where $\rho_s$is the superfluid electron number density) or $q_\nu h\rho_s d/M$ for a vortex in superfluid (where ρ_s is the superfluid atom number density). Here h and d are the Planck constant and the thickness of the sample (eg. the thickness of the superconductor film) respectively. Note that since a vortex motion under the Magnus force is similar to the motion of an electron in the presence of the magnetic field, the results obtained in this paper can than be directly used in the problem of an electron escaping provided that $\Omega = eB/M$ and $q_\nu$must be replaced by an electron charge e.

Eq.(1) can be explaned as fallows. The vector potential $\vec{A}$ reflects the existence of the vortex velocity dependent part(VVDP) of the Magnus force $\vec{F}_m = M\Omega(\vec{v}_s - \dot{\vec{r}}) \times \hat{z}$ which depends on the relative velocity between the superfluid velocity $\vec{v}_s$ (which is assumed without loss of generality to parallel to the x axis) and the

vortex velocity $\dot{\vec{r}}$. It is clear that the frequency dimensional parameter Ω we just have defined represents the strength of the Magnus force (or Lorenz force for the problem of an electron escaping). The superfluid velocity dependent part (SFVDP) of the Magnus force will contribute to the vortex potential $V(\vec{r})$. By following [1],we shall put the vortex potential $V(\vec{r})$, which contains both the contribution form SFVDP Magnus force and pinning centers, in the form

$$V(\vec{r}) = V_1(y) + \frac{1}{2}k_x x^2. \tag{2}$$

The pinning potential in x direction is approximated by harmonic potential characterized by parameter k_x. In this paper, the potential $V_1(y)$ consists of the contributions from the SFVDP Magnus force and the pinning potential in y direction is assumed to be of the metastable cubic-plus-quadratic form with metastable point at $y = 0$[2]. This metastable potential is characterized by two parameters: (i) ω_0, the frequency of the small oscillation about the metastable point $y = 0$ of the potential $V_1(y)$, and (ii) ω_b, the frequency of the small oscillation about $y = y_b$ ($V_1(y_b)$ is equal to the potential at the barrier top) of the inverted potential $-V_1(y)$. Note that, in the problem of an electron escaping, the potential $V_1(y)$ consists only the pinning potential in y direction since an electron can feel the Lorenz force by its own velocity. The last term in eq.(1) represents the dissipative environment of a vortex consisting of a set of harmonic oscillators as formulated in ref.[3]. The effect of the dissipative environment is specified by the spectral function

$$J(\omega) = \pi \sum_j \frac{c_j^2}{2m_j\omega_j}\delta(\omega - \omega_j). \tag{3}$$

In our problem of escaping, the Euclidean action corresponding to the Hamiltonian(1) is independent of the choice of gauge since the boundary condition $\vec{r}(0) = \vec{r}(\beta\hbar)$, where $\beta = 1/k_BT$ is the inverse temperature, is required. By this reason, we can choose any form of vector potential whenever it satisfies the relation $\vec{\nabla} \times \vec{A} = (M\Omega/q_\nu)\hat{z}$. As in ref.[1], the vector potential will be chosen in the form $\vec{A} = (M\Omega/q_\nu)(y, 0, 0)$. The Euclidean action corresponding to the Hamiltonian(1) with this form of the vector potential is[1]

$$\begin{aligned} S^E &= \int_0^{\beta\hbar} d\tau(\frac{1}{2}M|\dot{\vec{r}}|^2 + iM\Omega\dot{x}y + V_1(y) + \frac{1}{2}k_x x^2 + \sum_j[\frac{1}{2}m_j|\dot{\vec{q}_j}|^2 \\ &\quad + \frac{1}{2}m_j\omega_j^2|\vec{q}_j - \frac{c_j}{m_j\omega_j^2}\vec{r}|^2]). \end{aligned} \tag{4}$$

After integrating the environmental and x degrees of freedom of a vortex, the reduced thermodynamic description in the metastable direction (ie. y direction) can be known via the reduced partition function

$$Z_d = \oint \exp(-S^E_{eff}[y]/\hbar), \tag{5}$$

where

$$\begin{aligned} S^E_{eff}[y] &= \int_0^{\beta\hbar}(\frac{1}{2}M\dot{y}^2 + V_1(y))d\tau + \int_0^{\beta\hbar}\int_0^{\beta\hbar}[K(|\tau-\tau'|) + g(\tau-\tau')] \\ &\times[y(\tau) - y(\tau')]^2 d\tau' d\tau. \end{aligned} \tag{6}$$

From ref.[1], $K(\tau)$ and $g(\tau)$ are called normal and anomalous damping kernel respectively. They are expressed as

$$K(\tau) = \frac{1}{2\pi}\int_0^\infty d\omega J(\omega)\frac{\cosh[\omega(\beta\hbar/2-\tau)]}{\sinh[\omega\beta\hbar/2]}, \tag{7}$$

and

$$g(\tau) = \frac{M\Omega^2}{2\beta\hbar}\sum_{-\infty}^{\infty}(\frac{M\omega_x^2+\xi_n}{M\nu_n^2+M\omega_x^2+\xi_n})e^{i\nu_n\tau}. \tag{8}$$

Here

$$\xi_n = \frac{1}{\pi}\int_0^\infty d\omega\frac{J(\omega)}{\omega}\frac{2\nu_n^2}{\omega^2+\nu_n^2}; \nu_n = 2n\pi/\beta\hbar, \omega_x^2 = k_x/M. \tag{9}$$

In the problem of escaping, one of the important quantities is the escape rate. According to Afflect[4], the escape rate formula, denoted by K, is divided into two forms saperated by the crossover temperature, denoted by T_0, as follows.

$$K = -\frac{2}{\hbar}ImF \; ; for T < T_0, \tag{10}$$

and

$$K = -\frac{2}{\hbar}\frac{\beta}{\beta_0}ImF \; ; for T > T_0, \tag{11}$$

where $\beta_0 = 1/k_B T_0$ is the inverse crossover temperature, and F is the free energy which is related with the reduced partition function(5) by $Z_d = \exp(-\beta F)$. In eqs.(10) and (11), the imaginary part of the free energy, $ImF = -(1/\beta)Im(\ln Z_d)$, can be calculated by using the analytic continuation method pioneered by Langer[5]. Besides the free energy, another important quantity is the crossover temperature. It is the temperature where the change of dominating mechanism of the escape from thermal activation to quantum tunneling is roughly to occur. In the functional integral point of view[2], the crossover temperature is the temperature where the change of the dominant trajectory of the functional integral(5) from

the trivial trajectory ($y = 0$ and $y = y_b$) to the bounce trajectory (the back and forth trajectory in the inverted potential $-V_1(y)$) trajectory is to occur. In other words, if we decrease temperature from $T > T_0$ to $T < T_0$, then the corresponding dominant trajectory will be changed from trivial to bounce and the corresponding dominant physical mechnism of the escape process will roughly change from thermal activation to quantum tunneling.

Now, it is worth to find the equation for determining the crossover temperature T_0. The procedures are as follows. First, by the definition of crossover temperature, it is clear that slightly below T_0, the bounce trajectory will be replaced by the harmonic oscillator which is the small oscillation about y_b with the frequency $\omega_R = 2\pi/\beta_0\hbar$. Second, by using the variational principle $\delta S^E_{eff} = 0$ where δS^E_{eff} has already been defined in eq.(6), the equation of motion is obtained. Third, by substituting the harmonic oscillator solution from the first step into the equation of motion in the second step, then with the help of eqs.(7) and (8), one can linearize the equation of motion and get

$$\omega_R^2 + \omega_R \hat{\gamma}_M(\omega_R) = \omega_b^2, \tag{12}$$

where $\omega_R = 2\pi/\beta_0\hbar = 2\pi k_B T_0/\hbar$, $\omega_b^2 = -V''(y_b)/M$, and

$$\hat{\gamma}_M(x) = \hat{\gamma}(x) + \frac{\Omega^2 x}{x^2 + \omega_x^2 + x\hat{\gamma}(x)}, \ forall\ x \geq 0, \tag{13}$$

where $\hat{\gamma}(x) = (2x/M\pi)\int_0^\infty J(\omega)/\omega(\omega^2 - x^2)$ is the Laplace transform of the retarded friction[2], when the environment is represented by the Caldeira-Leggett model [3], which is related to ξ_n by $\xi_n = M|\nu_n|\hat{\gamma}(|\nu_n|)$. Note that $\hat{\gamma}_M(x)$, when the subscript M denotes the abbreviated name of Magnus force, reduces to $\hat{\gamma}(x)$ when the Magnus force is absent (i.e., $\hat{\gamma}_M \to \hat{\gamma}$ as $\Omega \to 0$) and then eq.(12) reduces to $\omega_R^2 + \omega_R\hat{\gamma}(\omega_R) = \omega_b^2$ [2] which is the equation for determining T_0 in the case of one dimensional system. This should not be a surprise since the additional term (the second term on the right hand side of eq.(13)), which is absent when $\Omega \to 0$, shows the effect on the crossover temperature from both the x degree of freedom via Ω and the environment via $\hat{\gamma}(x)$ while the first term shows only the effect from the environment.

Now, the interesting question is that how much can we know about the behavior of T_0 or equivalently ω_R. Clearly, to know all of its behaviors, one must find the roots of eq.(12). Unfortunately, it may be impossible to find them since $\hat{\gamma}(x)$ contains an integral over $J(\omega)$ which has no specific form in general cases. However, some of its properties can lead us to investigate some physical situations. The first property is the uniqueness of T_0. One can guess that if T_0 exists, then it should be unique since the crossover temperature is the temperature where the change of domination mechanism of the escape process is roughly to occur and once this change has occurred, it should not reoccur again. The second property

is the existence of T_0. One may guess at first sight that T_0 always exists because when we decrease the temperature form high to very low, then the dominating mechanism of escape process should roughly be changed from thermal activation to quantum tunneling at some temperature. These two properties can be proved mathematically by looking at eq.(12) carefully as follows. Rewriting eq.(12) as $x\hat{\gamma}_M(x) = \omega_b^2 - x^2$ (ω_R or T_0 is the root of this equation). Here, x is confined only in the positive range i.e., $x \geq 0$ since T_0 is the absolute temperature which is always greater than or equal to zero. Notice that $\omega_b^2 - x^2$ is the continuous decreasing function on positive range of x and has the maximum value equal to ω_b^2 at $x = 0$. Furthermore, one can prove from eq.(13), by differentiating $x\hat{\gamma}_M(x)$ that $x\hat{\gamma}_M(x)$ is a continuous increasing function on positive range of x. By these properties of $\omega_b^2 - x^2$ and $x\hat{\gamma}_M(x)$, it is clear that the root of the equation $x\hat{\gamma}_M(x) = \omega_b^2 - x^2$exists and is unique if and only if

$$\lim_{x\to 0} x\hat{\gamma}_M(x) \leq \omega_b^2. \tag{14}$$

Now, the two properties of T_0 mentioned earlier have already been proved. It can be summerized that the crossover temperature exists and is unique if the condition 14 is fulfilled. At this point, the following study of a vortex escaping will be divided into two cases.

First ($\omega_x \neq 0$) : In this case, one can prove from eq.(13) that $\lim_{x\to 0} x\hat{\gamma}_M(x) = 0 < \omega_b^2$ which implies by condition(14) that the unique crossover temperature T_0 always exists. The existence of T_0 tells us that (i) there is a temperature where the dominating mechanism of the escape process will be roughly changed, and (ii) the tunneling rate (the escape rate when the dominating mechanism is a quantum tunneling) is always nonzero because of the existence of bounce trajectory. In this case, the escape rate K for $T > T_0$ can be derived analytically by using the same methods in refs.[2] and [6] as follows. Replacing y by its Fourier series i.e., $y(\tau) = \sum_{n=-\infty}^{\infty} y_n e^{i\nu_n \tau}$ and substituting it into eq.(6) and developing $V_1(y)$ in a Taylor series around $y = 0$ and $y = y_b$, the semiclassical effective action about $y = 0$ (denoted by $S_{eff}^{E(0)}[y]$) and $y = y_b$ (denoted by $S_{eff}^{E(b)}[y]$) can be expressed in the form

$$S_{eff}^{E(0)}[y] = \frac{M\beta\hbar}{2}\lambda_0^{(0)} y_0^2 + M\beta\hbar \sum_{n=1}^{\infty} \lambda_n^{(0)} \left|y_n^2\right| ; \lambda_n^{(0)} = \nu_n^2 + \omega_0^2 + \nu_n \hat{\gamma}_M(\nu_n), \tag{15}$$

and

$$S_{eff}^{E(b)}[y] = V_b\beta\hbar + \frac{M\beta\hbar}{2}\lambda_0^{(b)} y_0^2 + M\beta\hbar \sum_{n=1}^{\infty} \lambda_n^{(b)} \left|y_n^2\right| ; \lambda_n^{(b)} = \nu_n^2 - \omega_b^2 + \nu_n \hat{\gamma}_M(\nu_n), V_b = V_1(y_b). \tag{16}$$

Splitting the reduced partition function(5) into the contributions arising from the Guassian fluctuations about trivial paths $y = 0$ and $y = y_b$ and write $Z_d = Z_d^{(0)} + Z_d^{(b)}$ where $Z_d^{(0)}$ and $Z_d^{(b)}$ are the reduced partition functions which have the corresponding effective action (15) and (16) respectively. After using the normalized functional measure in Fourier space[2] and Langer's thermodynamic method[5], the negative value of $\lambda_0^{(b)} = -\omega_b^2$ leads to an imaginary part of the free energy in the form

$$ImF = -\frac{\omega_0}{2\beta\omega_b}\left(\prod_{i=1}^{n}\frac{\lambda_n^{(0)}}{\lambda_n^{(b)}}\right)e^{-\beta V_b}. \tag{17}$$

Substituting eq.(17) into eq.(11), we obtain

$$K = \frac{\omega_0}{2\pi}\rho C_{qm}e^{-\beta V_b}, \tag{18}$$

where $\rho = \omega_R/\omega_b$ and $C_{qm} = \prod_{i=1}^{n}\lambda_n^{(0)}/\lambda_n^{(b)} \geq 1$ is called the quantum correction factor or quantum-mechanical enhancement factor because it describes the quantum effect (i.e., tunneling and increasing of average energy in the well) which enhances the escape rate.

Now, noticing from eq.(13) that $\hat{\gamma}_M$ increases as the Magnus force strength (characterized by Ω) increases. By this reason, one can conclude from eq.(12) that ω_R or ρ decreases when Magnus force strength increases and, by the definition of C_{qm} itself, C_{qm} also decreases when Magnus force strength increases. This implies that the VVDP Magnus force tends to decrease the escape rate. In contrast, the pinning potential in x direction tends to increase the escape rate since, from eq.(13), $\hat{\gamma}_M$ decreases as ω_x increases. Although these conclusions can be used when $T > T_0$ (because K in eq.(18) valid for $T > T_0$ only), it may be used when $T < T_0$ too. This stems from the fact that since the correction factor C_{qm} describes the quantum effect on the escape process including quantum tunneling, the effects of Magnus force and pinning potential in x direction on tunneling rate should be the same as on C_{qm}. As described above C_{qm} decreases (increascs) when Magnus force strength (pinning potential in x direction) increases. These imply (like in the case of $T > T_0$) that the VVDP Magnus force tends to decrease the tunneling rate while the pinning potential in x direction tends to increase the tunneling rate. Moreover, both pinning and dissipation tend to suppress the influence of the VVDP Magnus force on vortex escaping since Ω is in the numerator while ω_x and $\hat{\gamma}$ (which contains an integral over $J(\omega)$) are in the denominator of the second term of eq.(13).

Second ($\omega_x = 0$) : In this case, one can prove from eq.(13) that $\lim_{x\to 0} x\hat{\gamma}_M(x) = \Omega^2/[1+(2/M\pi)\int_0^\infty J(\omega)/\omega^3 d\omega]$. So, from condition(14), it is clear that the crossover temperature does not exist if

$$\frac{\Omega^2}{1+\frac{2}{M\pi}\int_0^\infty \frac{J(\omega)}{\omega^3}d\omega} > \omega_b^2. \tag{19}$$

Condition(19) tells us that the crossover temperature does not exist if the Magnus force strength is strong enough. This non-existence of crossover temperature implies that the bounce trajectory does not exist and, hence, the tunneling rate must vanish. Now, the interested question arises: Although the tunneling rate vanishes, is it possible that the escape process, when condition(19) is fulfilled, will be dominated by thermal activation over the entire range of temperature? The answer is no because of the fact that the value of $\lambda_0^{(b)}$ is now equal to $-\omega_b^2 + \Omega^2/[1 + (2/M\pi)\int_0^\infty J(\omega)/\omega^3 d\omega]$ (see eq.(16)) which is greater than zero when condition(19) is fulfilled. This positive value of $\lambda_0^{(b)}$ makes the free energy finite and real which implies that the escape rate must vanish or, equivalently, a vortex must be localized in the well. The above discussions can be summerized as follows. If $\omega_x = 0$ and the condition(19) is fulfilled, then the vortex must be localized in the well. Since the derivation of condition(19) is done irrelevance of temperature and dissipation, we will call condition(19) the localization criterion at finite temperature and dissipation. By using $M\omega_b^2 = -V''(y_b)$, the criterion(19) can be written in the form

$$\frac{(M\Omega)^2}{M+\frac{2}{\pi}\int_0^\infty \frac{J(\omega)}{\omega^3}d\omega} > |V''(y_b)|\,, \tag{20}$$

where, by the definition of Ω, $M\Omega$ is the mass independent parameter e.g., $M\Omega = h\rho_s d/2$ for a vortex in superconductor. Note that, for a vortex in superconductor, the localization criterion(20) reduces to the localization criterion in the case of no pinning at zero temperature given by P.Ao and D.J. Thouless[1] when the dissipation is absent i.e., $J(\omega) = 0$.In the case when the criterion(19) is violated, the escape rate, both for $T > T_0$ and $T < T_0$, does not vanish. The escape rate for $T > T_0$, denoted by $\tilde{K}$, in this case can be derived by using the same methods in the first case as

$$\tilde{K} = \frac{\omega_0}{2\pi}\tilde{\rho}C_{qm}e^{-\beta V_b}; \tilde{\rho} = \omega_{0M}\omega_R/\omega_0\omega_{bM}, \tag{21}$$

where

$$\omega_{0M}^2 = \omega_0^2 + \Omega^2/[1 + (2/M\pi)\int_0^\infty J(\omega)/\omega^3 d\omega,$$

and

$$\omega_{bM}^2 = \omega_b^2 - \Omega^2/[1 + (2/M\pi)\int_0^\infty J(\omega)/\omega^3 d\omega > 0.$$

The subscript M on ω_{0M} and ω_{bM} denotes the abbreviated name of Magnus force due to its effect via the parameter Ω. Note that $\omega_{0M} \to \omega_0$ and $\omega_{bM} \to \omega_b$ as $\Omega \to 0$ imply that $\tilde{K} \to K$ as $\Omega \to 0$. This should not be a surprise since in the absence of Magnus force, the x and y degree of freedoms are not coupled with

each other so the pinning potential in x direction characterized by ω_x has no effect on the escaping in the unstable direction i.e., y direction. Hence, the escape rate of the frist and second cases are identical and the localization criterion is always violated which implies that a vortex must escape from a mefastable potential with a specific nonvanishing escape rate at any temperature.

The above two cases show that the pinning potential in x direction is an important quantity because when $\omega_x \neq 0$, the escape rate is nonzero for any magnitude of the VVDP Magnus force while the escape rate for $\omega_x = 0$ is zero for strongly enough VVDP Magnus force. In other words, for $\omega_x = 0$, the strongly enough VVDP Magnus force renormalizes the original metastable potential to the stable one. In the classical point of view, ω_x can bend the trajectory of a vortex in such a way that it helps a vortex to escape from the well while the VVDP Magnus force tends to trap a vortex in the well by keeping it in a circular motion.

Now, we can define an effective mass of a vortex by using the localization criterion(20) as follows. Notice that the $M\Omega$ term in the numerator of (20) is mass independent, so the mass dependent term is only in the denominator. Hence, the effective mass (denoted by M^*) can be defined by

$$M^* = M + \frac{2}{\pi}\int_0^\infty \frac{J(\omega)}{\omega^3}d\omega, \tag{22}$$

and the criterion(20) becomes

$$\frac{(M\Omega)^2}{M^*} > |V''(y_b)|\,. \tag{23}$$

From criterion(23), the effective mass can be interpreted as follows. Since $M^* = M$ in the absence of dissipation (see eq.(22)), a damped vortex (a vortex in contact with the environment) behaves as if it is an undamped vortex (a vortex which is free from the environment) of the new bigger mass called an effective mass when it decides to escape from the pinning potential. This effective mass is equal to the original mass plus the extra mass originated from the environment since it depends on the spectral function. Note that this extra mass (the second term in the right hand side of eq.(22)) is proportional to the effective mass given by J.H. Han, P.Ao, and X.M.Zhu [7]. To understand more about the effective mass, we first consider the new masses μ_j and new coordinates $\vec{q}_j$ for the environment [8] given by

$$\vec{q}_j' = \frac{m_j\omega_j^2\vec{q}_j}{c_j}, \mu_j = \frac{c_j^2}{m_j\omega_j^4}. \tag{24}$$

From eq.(24), the Hamiltonian(1) can be rewritten as

$$H = \frac{1}{2M}|\vec{P} - q_\nu\vec{A}(\vec{r})|^2 + \sum_j \mu_j||\dot{\vec{q}}_j'|^2 + \omega_j^2|\vec{q}_j' - \vec{r}|^2]. \tag{25}$$

We can see that the model Hamiltonian(1), in fact, describes a vortex of mass M with many masses μ_j affected with spring to its coordinates $\vec{r}$. From eq.(3) and eq.(24), the sum of μ_j can be written in the form

$$\sum_j \mu_j = \frac{2}{\pi}\int_0^\infty \frac{J(\omega)}{\omega^3}d\omega. \tag{26}$$

Now, from eq.(22) and eq.(26), it is clear that the effective mass M^* is equal to the total mass of the system which is composed of a vortex of mass M with many masses μ_j. At this point, one may think that the coordinates of the effectively undamped vortex of mass M^* may be the center of mass coordinates which contain the total mass of the system. Although this conclusion may be possible, we can not exactly do so since our definition of the effective mass does not come directly from the dynamical approach (it is defined via the localization criterion). However, some conclusions can be made for the case of sufficiently weak environmental coupling so that $\sum_j \mu_j << M$. In this case, the center of mass coordinates of the system will approximately coincide with the original coordinates of a damped vortex at all time. By this reason, one can conclude in this case that the damped vortex of mass M can be effectively viewed as an undamped vortex of mass M^* and the coordinates of this undamped vortex is identical to the center of mass coordinates of the system which is approximately identical to the coordinates of an original damped vortex.

To summarize, we have studied the influence of pinning, dissipation, and Magnus force on vortex escaping when the potential, which contains both the contribution from SFVDP Magnus force and pinning potential in y direction, is modeled by the metastable cubic plus quadratic form and the pinning potential in x direction is approximated by the harmonic potential. The equation for determining the crossover temperature is derived. This equation leads us to define the localization criterion of a vortex at finite dissipation and temperature. The criterion shows that, at any temperature and dissipation, a vortex always escape from the well when the pinning potential in x direction is presented while it is localized in the well for strongly enough VVDP Magnus force when the pinning potential in x direction is absence. Moreover, this criterion also leads us to define the effective mass of a vortex in the sense that when a damped vortex decides to escape from the well, it can be effectively viewed as an undamped vortex of a new bigger mass called effective mass. The effective mass is equal to the original mass plus the extra mass originated from the environment and can be viewed as the total mass of the system when considering the system in the appropriate coordinates and masses. For sufficiently weak environmental coupling, the whole system can be effectively viewed as a one undamped vortex of effective mass, which is equal to the total mass of the system, described by the center of mass coordinates which approximately coincide with the coordinates of an original damped vortex. The escape rate formula is derived when the temperature is greater than the

crossover temperature and the pinning potential in x direction is nonzero. This escape rate formula and the equation for determining the crossover temperature allow us to make some conclusions about the role of pinning and dissipation on vortex escaping as follows. At any temperature, the VVDP Magnus force tends to decrease the escape rate while the pinning potential in x direction tends to increase the escape rate. Both pinning and dissipation tend to suppress the in fluence of the VVDP Magnus force on vortex escaping. The escape rate formula is also derived when the temperature is greater than the crossover temperature and the pinning potential in x direction is zero. In this case, the violation of localization criterion is required.

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BOSE-EINSTEIN CONDENSATION OF ATOMIC HYDROGEN

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A Thesis Submitted in Partial Fulfillment of the Requirements

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WATTANA LIM: BOSE-EINSTEIN CONDENSATION OF ATOMIC HYDROGEN THESIS ADVISOR: PROF. VIRULH SA-YAKANIT, F.D., 92 pp. ISBN 974-17-0269-8.

We study the ground state properties of Bose-Einstein condensation of atomic hydrogen in the Ioffe-Pritchard magnetic trap using many-body Feynman Path Integral theory, which leads to the calculation of the ground state energy and the wave function. We also calculate the size, peak condensate density and the value of the ground state energy, which are in fair agreement with the experimental results obtained by laser spectroscopy of 1S-2S transition.

Department Physics
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PATH INTEGRATION APPROACH TO CHARGED BOSONS IN AN ISOTROPIC TRAP

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A Thesis Submitted in Partial Fulfillment of the Requirements

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CHAKRIT NUALCHIMPLEE: PATH INTEGRATION APPROACH TO CHARGED BOSONS IN AN ISOTROPIC TRAP. THESIS ADVISOR: PROF. VIRULH SA-YAKANIT, F.D., 83 pp. ISBN 974-17-0273-6.

In this thesis, the case of charged bosons confined in an isotropic magnetic trap is studied by using Feynman path integration. We show that the upper bound of the ground state energy can be evaluated by applying the variational path integral technique. Consequently, the approximated density matrix and wavefunction are obtained. The ground state energy is then compared with the result obtained by Ginzburg – Pitaevskii – Gross approach. It is shown that our result agrees with such an approach. Furthermore, from our result, when we neglect the effect of screened Coulomb potential in the ground state energy of the screened Coulomb case, the ground state energy of the Coulomb potential arises as expected.

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สมบัติที่สถานะพื้นของอัลคาไลแก๊สที่ถูกกักแบบขึ้นกับทิศทาง โดยวิธีการอินทิเกรตตามวิถีของฟายน์แมน

นายณัฐพล นาคปฐมกุล

วิทยานิพนธ์นี้เป็นส่วนหนึ่งของการศึกษาตามหลักสูตรปริญญาวิทยาศาสตรมหาบัณฑิต
สาขาวิชาฟิสิกส์ ภาควิชาฟิสิกส์
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NATTHAPON NAKPATHOMKUN : GROUND-STATE PROPERTIES OF AN ANISOTROPICALLY TRAPPED ALKALI GAS USING FEYNMAN PATH INTEGRATION . THESIS ADVISOR : PROFESSOR VIRULH SA-YAKANIT, F. D., 98 pp. ISBN 974-17-0267-1.

The dilute weakly interacting alkali gas was shown to exhibit the phase transition called Bose-Einstein condensation for the first time in the experiment of Wieman's group in 1995. In this thesis, the ground state properties of the alkali gas trapped in an anisotropic magnetic field are investigated by using the variational method in path integral formalism. The interatomic interaction is approximated by the delta function which is short-range potential. The approximated density matrix is derived. Consequently the ground state energy and wavefunction are obtained. The ground state energy is then compared to the result obtained by the mean field approach both analytically and numerically. The result is shown to equivalent to the variational mean field approach. In addition, a comparison between path integral approach and the numerical mean field approach is shown to give no significant difference. The ground state wavefunction is extracted from the weighting function. Substitute the variational parameters into the expression of wavefunction one can see that the result is close to the numerical method.

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1 Response of the non-interacting Boson system under switching of the trap frequency

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Abstract

As a by-product of our attemp to make a theoretical description of the BOSENOVA in Non-interaction Bose gas, we found that the condensate density oscillates with time when we change the strength of the confinement potential. Some physical properties are calculated with discussions.

1.1 Introduction

In our attemps to simulate the phenomenon of implosion and explosion of the Interacting-Boson gas under switching of the "inteaction strength" or "scattering length" (BOSENOVA)[1] by the method of many-body Path Integrals, we found that the calculation is very complicate to find the time-evolution of the system if we want to add interaction terms between particles in the form of harmonic potential(the Harmonic Model[2]). Moreover, in the recent publications [3], many people have shown that the "three-body loss term" is needed in the Time-Dependent-Gross-Pitaevskii equation to describe correctly about this phenomenon (at least qualitatively). Hence our project still need some more works. Anyway, It is better to begin from some relatively simpler thing. Firstly, we found that the interactions between particles cause some calculation problem so we choose to remove it and retain the statistical correlations of the particles hoping that we can relagate this interaction to be included in the strength of the confining potential. Or in the other words, instead of switching the scattering length (as in the experimental results[1]) we switch the value of the trap frequency. By this way we can learn how the system behaves before embarking into the reallistic one which may be done by adding some corrections terms to the calculation.

1.2 The Time-Dependent Density Matrix (TDDM)

We start by looking at the time-evolution of the system of particles confined in harmonic potential under the changing of the frequency of the trap from $v \longrightarrow w$. For simplicity we assume the isotropy of the potential.($w_x = w_y = w_z$) . The time-dependent density matrix is

$$\rho_\beta(x,t|x') = \int\int K_w(x,it|x'')\,\rho_v(x'',\beta|x''')\,K_w(x''',-it|x')\,dx'''dx'', \quad (1)$$

where $\bar{x} = \{x_1, x_2, ..., x_N\}$

$$\rho_v(x'',\beta|x') = \left(\frac{v}{2\pi\sinh v\beta}\right)^{\frac{1}{2}} \exp\left(-\frac{v}{2}\frac{((x'')^2+(x')^2)\cosh v\beta - 2x'x''}{\sinh v\beta}\right),$$

$$K_w(x'',it|x') = \left(\frac{1}{2}\frac{w}{i\pi\sin wt}\right)^{\frac{1}{2}} \exp\left(-\frac{w}{2}\frac{((x'')^2+(x')^2)\cos wt - 2x'x''}{i\sin wt}\right).$$

we write in one dimension for convenience. The generalization to three dimension case is obvious. Hence

$$\rho_\beta(x,t|x') = \left(\frac{1}{8\pi^3}\frac{v}{\sinh v\beta}\frac{w^2}{\sin^2 wt}\right)^{\frac{1}{2}} \times \int\int \begin{pmatrix} \exp\left(\frac{wi}{2}\frac{\left(x^2+(x'')^2\right)\cos wt - 2xx''}{\sin wt}\right) \\ \exp\left(-\frac{v}{2}\frac{\left((x''')^2+(x'')^2\right)\cosh v\beta - 2x'''x''}{\sinh v\beta}\right) \\ \exp\left(-\frac{wi}{2}\frac{\left((x''')^2+(x')^2\right)(\cos wt) - 2x'''x'}{\sin wt}\right) \end{pmatrix} dx'''dx''.$$

the first integral can be done

$$= \left(\frac{1}{8\pi^3}\frac{vw^2}{\sin wt}\right)^{\frac{1}{2}} \left(\frac{2\pi}{(v\sin wt\cosh v\beta + wi\cos wt\sinh v\beta)}\right)^{\frac{1}{2}} \exp\left(i\frac{w}{2}\frac{\cos wt}{\sin wt}\left(x^2-(x')^2\right)\right)$$
$$\times \int dx'' \exp\begin{pmatrix} -\frac{1}{2}\frac{(v\cosh v\beta\sin wt - wi\cos wt\sinh v\beta)}{\sin wt\sinh v\beta}(x'')^2 - \frac{wi}{\sin wt}xx'' + \\ \frac{\sin wt\sinh v\beta}{2(v\cosh v\beta\sin wt + wi\cos wt\sinh v\beta)}\left(\frac{v^2(x'')^2}{\sinh^2 v\beta} - \frac{w^2(x')^2}{\sin^2 wt} + \frac{2vwix'x''}{\sinh v\beta\sin wt}\right) \end{pmatrix}$$

then do the second integral we have the final form of the time-dependent density matrix

$$\rho_\beta(x,t|x') = \left(\frac{vw^2}{2\pi\sinh v\beta\left(v^2\sin^2 wt + w^2\cos^2 wt\right)}\right)^{\frac{1}{2}} \times \exp\left[-\frac{w}{2}\frac{\left[i\left(v^2-w^2\right)\sinh v\beta\cos wt\sin wt + wv\cosh v\beta\right](x')^2 + \left[-i\left(v^2-w^2\right)\sin w\cos wt\sinh v\beta + vw\cosh v\beta\right]x^2 - 2vwxx'}{\left(v^2\sin^2 wt + w^2\cos^2 wt\right)\sinh v\beta}\right] \quad (2)$$

1.3 Density of Particles

the fourier transform of the density for distinguishable particles can be found easily

$$\left\langle e^{iqx}\right\rangle = \frac{\int\rho_\beta(x,t|x)\,e^{iqx}dx}{\int\rho_\beta(x,t|x)\,dx} = \exp\left(-q^2\frac{\cosh\frac{1}{2}v\beta}{\sinh\frac{1}{2}v\beta}\frac{v^2\sin^2 wt + w^2\cos^2 wt}{4vw^2}\right). \quad (3)$$

where

$$n(x,t) = \frac{1}{2\pi}\int dq e^{-iqx}\left\langle e^{iqx}\right\rangle$$

Then the density of particle for distinguishable particles can be calculate

$$n(x) = \sqrt{\frac{vw^2}{\pi\left(v^2\sin^2 wt + w^2\cos^2 wt\right)}\frac{\sinh\frac{1}{2}v\beta}{\cosh\frac{1}{2}v\beta}}\exp\left(-x^2\frac{vw^2}{v^2\sin^2 wt + w^2\cos^2 wt}\frac{\sinh\frac{1}{2}v\beta}{\cosh\frac{1}{2}v\beta}\right). \quad (4)$$

For the case of identical particles, the permutation sum can be applied in the same way as [2]. This case is even simpler because there is no center of mass coordinates. We can write in three dimension,

$$n_{\mathbf{q}} = \frac{1}{N}\sum_{M_1..M_N}\sum_\alpha \alpha M_\alpha\mathcal{K}_\alpha(\mathbf{q})\frac{1}{M_\alpha!\alpha^{M_\alpha}}\mathcal{K}_\alpha^{M_\alpha-1}\prod_{\gamma\neq\alpha}\frac{1}{M_\gamma!\gamma^{M_\gamma}}\mathcal{K}_\gamma^{M_\gamma} \quad (5)$$

where

$$\mathcal{K}_\gamma = \int d\mathbf{r}_{\gamma+1}...\int d\mathbf{r}_1\delta(\mathbf{r}_{\gamma+1}-\mathbf{r}_1)\prod_{j=1}^{\gamma}\rho_\beta(\mathbf{r}_{j+1},t,\beta|\mathbf{r}_j,0) \quad (6)$$

and

$$\mathcal{K}_\gamma(\mathbf{q}) = \int d\mathbf{r}_{\gamma+1}...\int d\mathbf{r}_1\delta(\mathbf{r}_{\gamma+1}-\mathbf{r}_1)\,e^{i\mathbf{q}\cdot\mathbf{r}_s}\prod_{j=1}^{\gamma}\rho_\beta(\mathbf{r}_{j+1},t,\beta|\mathbf{r}_j,0) \quad (7)$$

the 1-particle TDDM satisfy the semigroup property so we can easily replace the imaginary time β by $\gamma\beta$ for the cycly of length γ. Then we can evaluate 6

$$\mathcal{K}_\gamma = \int d\mathbf{r}_{\gamma+1} ... \int d\mathbf{r}_1 \delta\left(\mathbf{r}_{\gamma+1} - \mathbf{r}_1\right) \prod_{j=1}^{\gamma} \rho_\beta\left(\mathbf{r}_{j+1}, t, \beta | \mathbf{r}_j, 0\right) = \left(\frac{1}{2\sinh\frac{\gamma v\beta}{2}}\right)^3$$

For $\mathcal{K}_\gamma(\mathbf{q})$, we have to consider

$$\mathcal{K}_\gamma(\mathbf{q}) = \int d\mathbf{r}_{\gamma+1} ... \int d\mathbf{r}_1 \delta\left(\mathbf{r}_{\gamma+1} - \mathbf{r}_1\right) \boxed{e^{i\mathbf{q}\cdot\mathbf{r}_\delta}} \prod_{j=1}^{\gamma} \rho_\beta\left(\mathbf{r}_{j+1}, t, \beta | \mathbf{r}_j, 0\right)$$

however, the position of $\mathbf{r}_\delta$ is not important in this expectation value. Hence we can write,

$$= \int d\mathbf{r}_{\gamma+1} ... \int d\mathbf{r}_3 \int d\mathbf{r}_1 \delta\left(\mathbf{r}_{\gamma+1} - \mathbf{r}_1\right) \rho_\beta\left(\mathbf{r}_{\gamma+1}, t, \beta | \mathbf{r}_\gamma, 0\right) \rho_\beta\left(\mathbf{r}_\gamma, t, \beta | \mathbf{r}_{\gamma-1}, 0\right) ...$$
$$...\rho_\beta\left(\mathbf{r}_4, t, \beta | \mathbf{r}_3, 0\right) \int d\mathbf{r}_2 \rho_\beta\left(\mathbf{r}_3, t, \beta | \mathbf{r}_2, 0\right) \boxed{e^{i\mathbf{q}\cdot\mathbf{r}_2}} \rho_\beta\left(\mathbf{r}_2, t, \beta | \mathbf{r}_1, 0\right)$$

using semi-group property

$$\begin{aligned}
\mathcal{K}_\gamma(\mathbf{q}) &= \int d\mathbf{r}_1 \int d\mathbf{r}_2 \int d\mathbf{r}_3 \rho_\beta\left(\mathbf{r}_1, t, (\gamma-2)\beta | \mathbf{r}_3, 0\right) \rho_\beta\left(\mathbf{r}_3, t, \beta | \mathbf{r}_2, 0\right) \boxed{e^{i\mathbf{q}\cdot\mathbf{r}_2}} \rho_\beta\left(\mathbf{r}_2, t, \beta | \mathbf{r}_1, 0\right) \\
&= \int d\mathbf{r}_1 \int d\mathbf{r}_2 \rho_\beta\left(\mathbf{r}_1, t, (\gamma-1)\beta | \mathbf{r}_2, 0\right) \boxed{e^{i\mathbf{q}\cdot\mathbf{r}_2}} \rho_\beta\left(\mathbf{r}_2, t, \beta | \mathbf{r}_1, 0\right) \\
&= \int d\mathbf{r}_2 \int d\mathbf{r}_1 \rho_\beta\left(\mathbf{r}_2, t, \beta + (\gamma-1)\beta | \mathbf{r}_1, (\gamma-1)\beta\right) \rho_\beta\left(\mathbf{r}_1, t, (\gamma-1)\beta | \mathbf{r}_2, 0\right) \boxed{e^{i\mathbf{q}\cdot\mathbf{r}_2}} \\
&= \int d\mathbf{r}_2 \rho_\beta\left(\mathbf{r}_2, t, \gamma\beta | \mathbf{r}_2, 0\right) \boxed{e^{i\mathbf{q}\cdot\mathbf{r}_2}}
\end{aligned}$$

Finally,

$$\begin{aligned}
\mathcal{K}_\gamma(\mathbf{q}) &= \int d\mathbf{r}_2 \rho_\beta\left(\mathbf{r}_2, t, \gamma\beta | \mathbf{r}_2, 0\right) \boxed{e^{i\mathbf{q}\cdot\mathbf{r}_2}} \\
&= \left[\left(\frac{vw^2}{2\pi\left(v^2\sin^2 wt + w^2\cos^2 wt\right)\sinh\gamma v\beta}\right)^{\frac{1}{2}} \int dx \exp\left[-\frac{vw^2\tanh\frac{\gamma v\beta}{2}}{\left(v^2\sin^2 wt + w^2\cos^2 wt\right)}x^2 + iq\right.\right. \\
&= \left(\frac{1}{2\sinh\frac{\gamma v\beta}{2}}\right)^3 \exp\left[-\mathbf{q}^2\frac{\left(v^2\sin^2 wt + w^2\cos^2 wt\right)}{4vw^2\tanh\frac{\gamma v\beta}{2}}\right]
\end{aligned}$$

with normalization, from 5

$$
\begin{aligned}
n_{\mathbf{q}} &= \frac{1}{NZ_I}\sum_{M_1..M_N}\sum_{\alpha}\alpha M_\alpha \mathcal{K}_\alpha(\mathbf{q})\frac{1}{M_\alpha!\alpha^{M_\alpha}}\mathcal{K}_\alpha^{M_\alpha-1}\prod_{\gamma\neq\alpha}\frac{1}{M_\gamma!\gamma^{M_\gamma}}\mathcal{K}_\gamma^{M_\gamma} \\
&= \frac{1}{NZ_I}\sum_{M_1..M_N}\sum_{\alpha}\alpha M_\alpha\left(\frac{1}{2\sinh\frac{\alpha v\beta}{2}}\right)^3\exp\left[-\mathbf{q}^2\frac{\left(v^2\sin^2 wt+w^2\cos^2 wt\right)}{4vw^2\tanh\frac{\alpha v\beta}{2}}\right] \\
&\quad\times\frac{1}{M_\alpha!\alpha^{M_\alpha}}\left(\frac{1}{2\sinh\frac{\alpha v\beta}{2}}\right)^{3(M_\alpha-1)}\prod_{\gamma\neq\alpha}\frac{1}{M_\gamma!\gamma^{M_\gamma}}\left(\frac{1}{2\sinh\frac{\gamma v\beta}{2}}\right)^{3M_\gamma} \\
&= \frac{1}{NZ_I}\sum_{M_1..M_N}\sum_{\gamma}\gamma M_\gamma\exp\left[-\mathbf{q}^2\frac{\left(v^2\sin^2 wt+w^2\cos^2 wt\right)}{4vw^2\tanh\frac{\gamma v\beta}{2}}\right]\prod_{\gamma\neq\alpha}\frac{1}{M_\gamma!\gamma^{M_\gamma}}\left(\frac{1}{2\sinh\frac{\gamma v\beta}{2}}\right)^{3M_\gamma}
\end{aligned}
$$

To remove the constraint $\sum_\gamma \gamma M_\gamma = N$ we have to introduce the generating function

$$\mathcal{G}_1(u,\mathbf{q}) = \sum_{N=0}^{\infty}\left[Z_I(N)\,N n_{\mathbf{q}}\right]u^N$$

which can be written

$$
\begin{aligned}
\mathcal{G}_1(u,\mathbf{q}) &= \sum_{N=0}^{\infty}\sum_{M_1..M_N}\sum_{\gamma}\gamma M_\gamma\exp\left[-\mathbf{q}^2\frac{\left(v^2\sin^2 wt+w^2\cos^2 wt\right)}{4vw^2\tanh\frac{\gamma v\beta}{2}}\right]\prod_{\gamma}\frac{1}{M_\gamma!}\left(\frac{u^\gamma}{\gamma\left(2\sinh\frac{\gamma v\beta}{2}\right)^3}\right)^{M_\gamma} \\
&= \sum_{M=0}^{\infty}\sum_{\gamma=1}^{\infty}\gamma\exp\left[-\mathbf{q}^2\frac{\left(v^2\sin^2 wt+w^2\cos^2 wt\right)}{4vw^2\tanh\frac{\gamma v\beta}{2}}\right]\left(\frac{u^\gamma}{\gamma\left(2\sinh\frac{\gamma v\beta}{2}\right)^3}\right) \\
&\quad\times\prod_{\gamma=1}^{\infty}\frac{1}{(M_\gamma-1)!}\left(\frac{u^\gamma}{\gamma\left(2\sinh\frac{\gamma v\beta}{2}\right)^3}\right)^{(M_\gamma-1)} \\
&= \sum_{\gamma=1}^{\infty}\exp\left[-\mathbf{q}^2\frac{\left(v^2\sin^2 wt+w^2\cos^2 wt\right)}{4vw^2}\coth\frac{\gamma v\beta}{2}\right]\left(\frac{u^\gamma}{\left(2\sinh\frac{\gamma v\beta}{2}\right)^3}\right) \\
&\quad\times\sum_{M=0}^{\infty}\prod_{\gamma=1}^{\infty}\frac{1}{(M_\gamma-1)!}\left(\frac{u^\gamma}{\gamma\left(2\sinh\frac{\gamma v\beta}{2}\right)^3}\right)^{(M_\gamma-1)} \\
&= \Xi(u)\sum_{\gamma=1}^{\infty}\exp\left[-\mathbf{q}^2\frac{\left(v^2\sin^2 wt+w^2\cos^2 wt\right)}{4vw^2}\coth\frac{\gamma v\beta}{2}\right]\left(\frac{u^\gamma}{\left(2\sinh\frac{\gamma v\beta}{2}\right)^3}\right)
\end{aligned}
$$

where

$$\Xi(u) = \sum_{M=0}^{\infty}\prod_{\gamma=1}^{\infty}\frac{1}{(M_\gamma-1)!}\left(\frac{u^\gamma}{\gamma\left(2\sinh\frac{\gamma v\beta}{2}\right)^3}\right)^{(M_\gamma-1)}$$

$$= \exp\left[\sum_{\gamma=1}^{\infty}\frac{u^\gamma}{\gamma\left(2\sinh\frac{\gamma v\beta}{2}\right)^3}\right] \tag{8}$$

is the generating function for the partition function of N identical particles as found in [2].

the Fourier transform of the density can be found from this generating function

$\frac{1}{N!}\frac{d^N}{du^N}\mathcal{G}_1(u,\mathbf{q})|_{u=0} = \frac{1}{N!}\frac{d^N}{du^N}\sum_{N=0}^{\infty}[Z_I(N)Nn_{\mathbf{q}}]u^N|_{u=0} = n_{\mathbf{q}}$

then

$$n_{\mathbf{q}} = \frac{1}{N!}\frac{d^N}{du^N}\left[\Xi(u)\sum_{\gamma=1}^{\infty}\exp\left[-\mathbf{q}^2\frac{\left(v^2\sin^2 wt + w^2\cos^2 wt\right)}{4vw^2}\coth\frac{\gamma v\beta}{2}\right]\left(\frac{u^\gamma}{\left(2\sinh\frac{\gamma v\beta}{2}\right)^3}\right)\right]_{u=0}$$

$$n_{\mathbf{q}} = \frac{1}{N}\sum_{\gamma=1}^{N}\frac{\exp\left[-\mathbf{q}^2\frac{\left(v^2\sin^2 wt+w^2\cos^2 wt\right)}{4vw^2}\coth\frac{\gamma v\beta}{2}\right]}{\left(2\sinh\frac{\gamma v\beta}{2}\right)^3}\frac{Z_I(N-\gamma)}{Z_I(N)} \tag{9}$$

then, the spatial density distribution can be found by

$n(\mathbf{r}) = \frac{1}{N}\left\langle\sum_{\alpha=1}^{N}\delta(\mathbf{r}-\mathbf{r}_\alpha)\right\rangle_I = \int\frac{d\mathbf{q}}{(2\pi)^3}n_{\mathbf{q}}e^{-i\mathbf{q}\cdot\mathbf{r}}$

$= \frac{1}{N}\sum_{\gamma=1}^{N}\frac{1}{\left(2\sinh\frac{\gamma v\beta}{2}\right)^3}\frac{Z_I(N-\gamma)}{Z_I(N)}\int\frac{d\mathbf{q}}{(2\pi)^3}\exp\left[-\mathbf{q}^2\frac{\left(v^2\sin^2 wt+w^2\cos^2 wt\right)}{4vw^2}\coth\frac{\gamma v\beta}{2} - i\mathbf{q}\cdot\mathbf{r}\right]$

$= \frac{1}{N}\sum_{\gamma=1}^{N}\frac{1}{\left(2\sinh\frac{\gamma v\beta}{2}\right)^3}\frac{Z_I(N-\gamma)}{Z_I(N)}\left(\frac{vw^2\tanh\frac{\gamma v\beta}{2}}{\pi(v^2\sin^2 wt+w^2\cos^2 wt)}\right)^{\frac{3}{2}}\exp\left[-\mathbf{r}^2\frac{vw^2\tanh\frac{\gamma v\beta}{2}}{(v^2\sin^2 wt+w^2\cos^2 wt)}\right]$

$\equiv \frac{1}{N}\sum_{\gamma=1}^{N}\frac{Z_I(N-\gamma)}{Z_I(N)}\frac{e^{-\frac{\gamma v\beta}{2}}}{(1-e^{-\gamma v\beta})^3}\left(\frac{w}{\pi}\mathbb{A}_\gamma\right)^{\frac{3}{2}}\exp\left[-w\mathbb{A}_\gamma\mathbf{r}^2\right]$

where

$$\mathbb{A}_\gamma = \frac{vw\tanh\frac{\gamma v\beta}{2}}{\left(v^2\sin^2 wt + w^2\cos^2 wt\right)}$$

we define $\mathbb{A}_\gamma$ to be a dimesionless quantity)

and we define $b = e^{-\frac{v\beta}{2}}$

$$n(\mathbf{r}) = \frac{1}{N}\sum_{\gamma=1}^{N} \frac{Z_I(N-\gamma)}{Z_I(N)} \frac{b^{\frac{3\gamma}{2}}}{(1-b^{\gamma})^3} \left(\frac{w}{\pi}\mathbb{A}_\gamma\right)^{\frac{3}{2}} \exp\left[-w\mathbb{A}_\gamma \mathbf{r}^2\right] \tag{10}$$

Now we see that the result is resemble the one from the work by FB,JTD and LFL except the modification of the factor $\mathbb{A}_\gamma$. Note that $\mathbb{A}_\gamma$ is a "Numerically" finite function of temperature and time. Since the formula 10 is not useful for numerical calculation, we apply the following techniques (I took from Sven's note)

1.3.1 Recursion relation for Partition funtion

$$\mathbb{Z}_I(N) = \frac{1}{N}\sum_{m=0}^{N-1} \frac{b^{\frac{3}{2}(N-m)}}{\left(1-b^{(N-m)}\right)^3} \mathbb{Z}_I(m) \tag{11}$$

because the factor $\frac{b^{\frac{3}{2}(N-m)}}{\left(1-b^{-(N-m)}\right)}$ is very small and impractical for numerical calculation so we single it out and define an object

$$\frac{\mathbb{Z}_I(N)}{\mathbb{Z}_I(N-1)} = \rho(N)\, b^{\frac{3}{2}} \tag{12}$$

then we can find

$$\begin{aligned}
\frac{\mathbb{Z}_I(N)}{\mathbb{Z}_I(m)} &= \frac{\mathbb{Z}_I(N)}{\mathbb{Z}_I(N-1)} \frac{\mathbb{Z}_I(N-1)}{\mathbb{Z}_I(N-2)} \cdots \frac{\mathbb{Z}_I(m+1)}{\mathbb{Z}_I(m)} \\
&= \rho(N)\, b^{\frac{3}{2}} \rho(N-1)\, b^{\frac{3}{2}} \ldots \rho(m+1)\, b^{\frac{3}{2}} \\
\frac{\mathbb{Z}_I(N)}{\mathbb{Z}_I(k)} &= b^{\frac{3}{2}(N-k)} \prod_{j=k+1}^{N} \rho(j)
\end{aligned} \tag{13}$$

from 12 we can find $\rho(1)$

$$\rho(1) = b^{-\frac{3}{2}} \frac{\mathbb{Z}_I(1)}{\mathbb{Z}_I(0)} = b^{-\frac{3}{2}} \frac{b^{\frac{3}{2}}}{(1-b)^3} = \frac{1}{(1-b)^3}$$

the next activity can be proceeded from 13 and 11

$$\begin{aligned}
\rho(2) &= b^{-\frac{3}{2}} \frac{\mathbb{Z}_I(2)}{\mathbb{Z}_I(1)} = \frac{b^{-\frac{3}{2}}}{\mathbb{Z}_I(1)} \frac{1}{2} \sum_{m=0}^{1} \frac{b^{\frac{3}{2}(2-m)}}{\left(1-b^{(2-m)}\right)^3} \mathbb{Z}_I(m) \\
&= \frac{1}{2}\left[\frac{1}{(1-b^2)^3}\frac{1}{\rho(1)} + \frac{1}{(1-b)^3}\right]
\end{aligned}$$

$$\begin{aligned}\rho(3) &= b^{-\frac{3}{2}}\frac{\mathbb{Z}_I(3)}{\mathbb{Z}_I(2)} = \frac{b^{-\frac{3}{2}}}{\mathbb{Z}_I(2)}\frac{1}{3}\sum_{m=0}^{2}\frac{b^{\frac{3}{2}(3-m)}}{\left(1-b^{(3-m)}\right)^3}\mathbb{Z}_I(m)\\ &= \frac{1}{3}\left[\left(\frac{1}{\left(1-b^{(3)}\right)^3}\frac{1}{\rho(1)}+\frac{1}{\left(1-b^{(2)}\right)^3}\right)\frac{1}{\rho(2)}+\frac{1}{(1-b)^3}\right]\end{aligned}$$

$$\begin{aligned}\rho(4) &= \frac{1}{4}\left[\frac{1}{\left(1-b^{(4)}\right)^3}\frac{1}{\rho(1)\rho(2)\rho(3)}+\frac{1}{\left(1-b^{(3)}\right)^3}\frac{1}{\rho(2)\rho(3)}+\frac{1}{\left(1-b^{(2)}\right)^3}\frac{1}{\rho(3)}+\frac{1}{(1-b)^3}\right]\\ &= \frac{1}{4}\left[\left(\left(\frac{1}{\left(1-b^{(4)}\right)^3}\frac{1}{\rho(1)}+\frac{1}{\left(1-b^{(3)}\right)^3}\right)\frac{1}{\rho(2)}+\frac{1}{\left(1-b^{(2)}\right)^3}\right)\frac{1}{\rho(3)}+\frac{1}{(1-b)^3}\right]\end{aligned}$$

$$\begin{aligned}\rho(5) &= \frac{1}{5}\left[\begin{array}{c}\frac{1}{\left(1-b^{(5)}\right)^3}\frac{1}{\rho(1)\rho(2)\rho(3)\rho(4)}+\frac{1}{\left(1-b^{(4)}\right)^3}\frac{1}{\rho(2)\rho(3)\rho(4)}+\frac{1}{\left(1-b^{(3)}\right)^3}\frac{1}{\rho(3)\rho(4)}\\ +\frac{1}{\left(1-b^{(2)}\right)^3}\frac{1}{\rho(3)}+\frac{1}{(1-b)^3}\end{array}\right]\\ &= \frac{1}{5}\left[\begin{array}{c}\left(\left(\left(\frac{1}{\left(1-b^{(5)}\right)^3}\frac{1}{\rho(1)}+\frac{1}{\left(1-b^{(4)}\right)^3}\right)\frac{1}{\rho(2)}+\frac{1}{\left(1-b^{(3)}\right)^3}\right)\frac{1}{\rho(4)}+\frac{1}{\left(1-b^{(2)}\right)^3}\right)\frac{1}{\rho(3)}\\ +\frac{1}{(1-b)^3}\end{array}\right]\end{aligned}$$

Let call

$$\xi(j) \equiv \frac{1}{\left(1-b^j\right)^3}$$

then the formula is

$$\rho(N) = \frac{1}{N}\left(\xi(1)+\sum_{l=2}^{N}\xi(l)\prod_{k=N+1-l}^{N-1}\frac{1}{\rho(k)}\right) \tag{14}$$

Now we can find the recursion relation for the Density

$$n(\mathbf{r}) = \frac{1}{N}\sum_{\gamma=1}^{N}\frac{Z_I(N-\gamma)}{Z_I(N)}\frac{b^{\frac{3\gamma}{2}}}{\left(1-b^{\gamma}\right)^3}\left(\frac{w}{\pi}\mathbb{A}_\gamma\right)^{\frac{3}{2}}\exp\left[-w\mathbb{A}_\gamma\mathbf{r}^2\right] \tag{15}$$

from 13

$$\frac{\mathbb{Z}_I(N)}{\mathbb{Z}_I(k)} = b^{\frac{3}{2}(N-k)}\prod_{j=k+1}^{N}\rho(j) \Rightarrow \frac{\mathbb{Z}_I(N-\gamma)}{\mathbb{Z}_I(N)} = b^{-\frac{3}{2}\gamma}\prod_{j=N-\gamma+1}^{N}\frac{1}{\rho(j)}$$

then

$$
\begin{aligned}
n(\mathbf{r}) &= \frac{1}{N}\sum_{\gamma=1}^{N}\frac{1}{(1-b^{\gamma})^{3}}\left(\frac{w}{\pi}\mathbb{A}_{\gamma}\right)^{\frac{3}{2}}\exp\left[-w\mathbb{A}_{\gamma}\mathbf{r}^{2}\right]\left(\prod_{j=N-\gamma+1}^{N}\frac{1}{\rho(j)}\right)\\
&\equiv \frac{1}{N}\sum_{\gamma=1}^{N}a_{\gamma}\left(\prod_{j=N-\gamma+1}^{N}\frac{1}{\rho(j)}\right)
\end{aligned}
$$

where

$$
\begin{aligned}
\mathbb{A}_{\gamma} &= \frac{vw\tanh\frac{\gamma v\beta}{2}}{\left(v^{2}\sin^{2}wt+w^{2}\cos^{2}wt\right)}\\
a_{\gamma} &= \frac{1}{(1-b^{\gamma})^{3}}\left(\frac{w}{\pi}\mathbb{A}_{\gamma}\right)^{\frac{3}{2}}\exp\left[-w\mathbb{A}_{\gamma}\mathbf{r}^{2}\right]
\end{aligned}
$$

$$
n(\mathbf{r},t)=\frac{1}{N}\frac{a(1)+\cfrac{a(2)+\cfrac{a(3)+\ldots+\cfrac{a(N-1)+\frac{a(N)}{\rho(1)}}{\rho(2)}}{\rho(N-2)}}{\rho(N-1)}}{\rho(N)} \tag{16}
$$

This formula 16 can be calculated easily and some result can be shown

Perturbation Theory for the Distinguishable Particles in switching harmonic trap

-Our system is particles confined in harmonic potential interact with some kind of 2 paticles potential for example, contact potential or s-wave scattering interaction, Morse Potential, etc.

-What we are interested is the evolution of the system after abruptly changing the confining potential from v to w.

-We have already found the density matrix and particle density for the *non-interacting* particles under harmonic potential, the number density of the system oscillate with frequency $2w$. Note that this is a zero order of the perturbation theory of our system.

-In real experimental results the condensate is oscillated and damped down due to the interaction between the condensate and the thermal cloud.

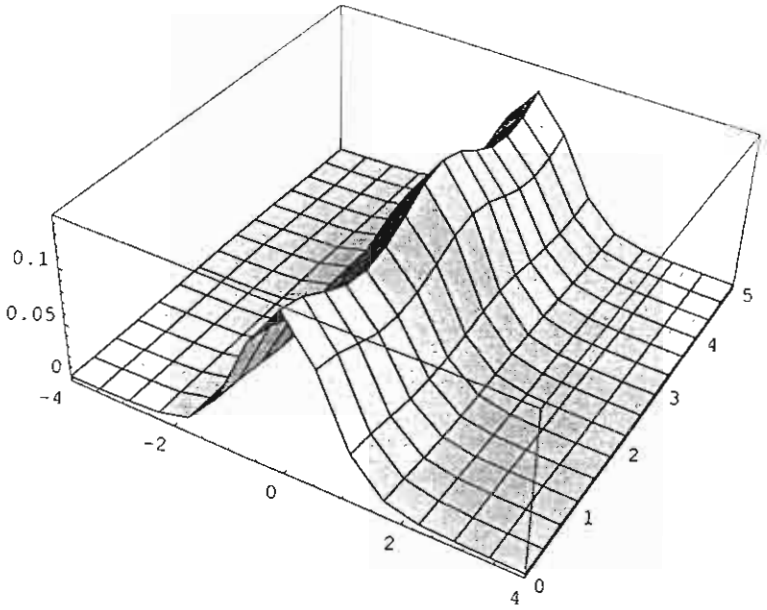

Figure 1: v=1 w=2 N=200

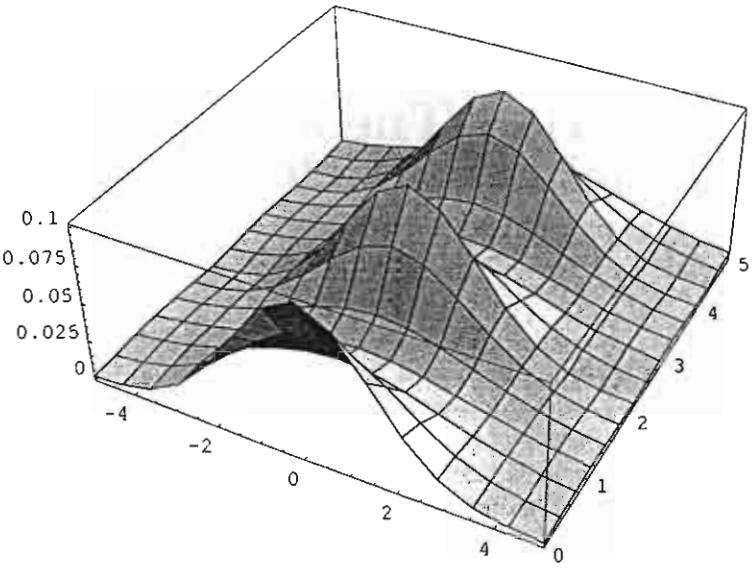

Figure 2: v=1 w=1.1 N=200

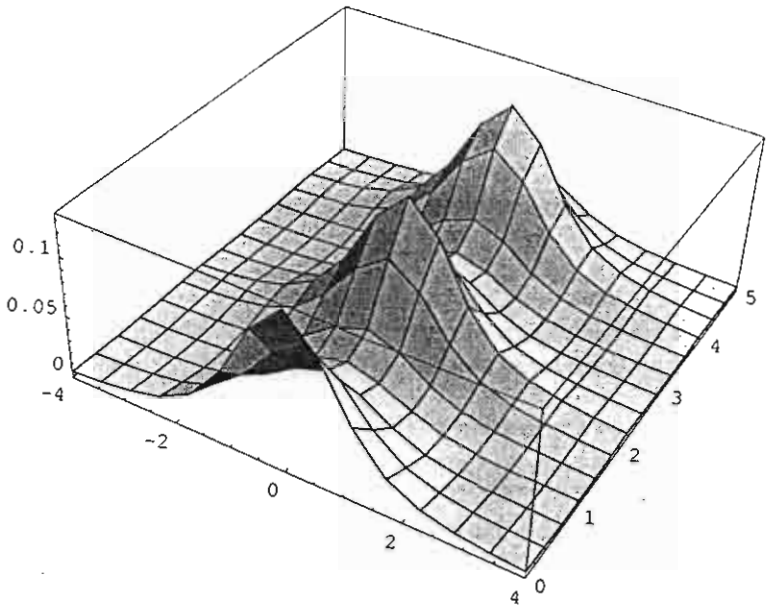

Figure 3: v=1 w=1.01 for N=200

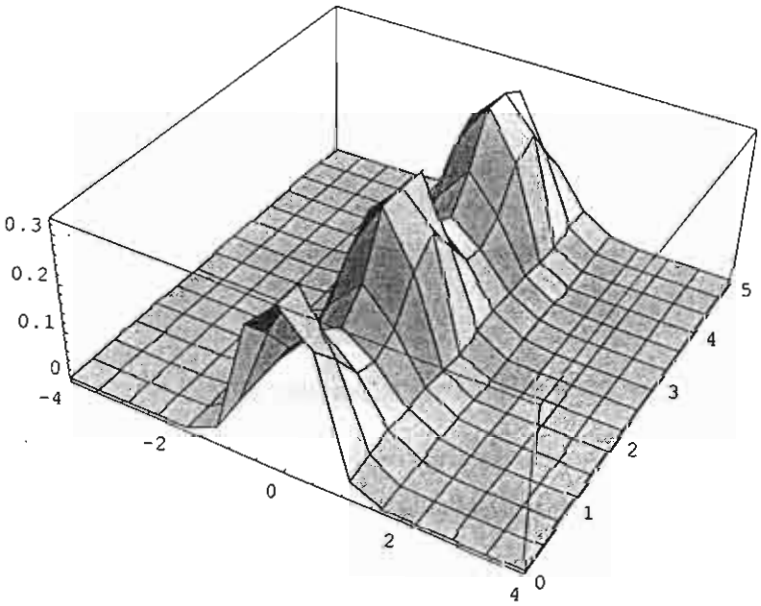

Figure 4: v=1 w=1.5 N=1000

-We would like to see how the *interaction* modified the oscillation of the system, will the oscillation damped?

-We would like to see how the *statistics* modified the oscillation of the system, quantitatively.

1.3.2 First Order Approximation

The Time-Dependent Density Matrix

$$\begin{aligned}\rho(t,\beta) &= \left[\mathcal{T}\exp\left[-i\int_0^t dt'\,(H_w+V)\right]\right]\left[\mathcal{T}\exp\left[-\int_0^\beta d\tau\,(H_v+V)\right]\right] \\ &\quad\times\left[\mathcal{T}\exp\left[-i\int_0^t dt'\,(H_w+V)\right]\right]^\dagger \qquad (17)\end{aligned}$$

To first order perturbation,

$\left[\mathcal{T}\exp\left[-i\int_0^t dt'\,(H_w+V)\right]\right] \simeq e^{-i\int_0^t dt' H_w} - i\int_0^t dt'\mathcal{T}\left(Ve^{-i\int_0^t dt'' H_w}\right)$

$\left[\mathcal{T}\exp\left[-i\int_0^\beta d\tau\,(H_v+V)\right]\right] \simeq e^{-\int_0^\beta d\tau H_v} - \int_0^\beta d\tau\mathcal{T}\left(Ve^{-\int_0^\beta d\tau' H_v}\right)$

Substitute into 17 and keep only first order in V, because none of the Hermiltonian or the potential are time dependent,

$$\begin{aligned}&\left[e^{-i\int_0^t dt' H_w} - i\int_0^t dt'\mathcal{T}\left(Ve^{-i\int_0^t dt'' H_w}\right)+...\right]\left[e^{-\int_0^\beta d\tau H_v} - \int_0^\beta d\tau\mathcal{T}\left(Ve^{-\int_0^\beta d\tau' H_v}\right)+...\right] \\ &\times\left[e^{i\int_0^t dt' H_w} + i\int_0^t dt'\mathcal{T}\left(Ve^{i\int_0^t dt'' H_w}\right)+...\right] \\ &\simeq\left[e^{-itH_w} - i\int_0^t dt' e^{-i(t-t')H_w}Ve^{-it'H_w}\right]\left[e^{-\beta H_v} - \int_0^\beta d\tau e^{-(\beta-\tau)H_v}Ve^{-\tau H_v}+...\right] \\ &\times\left[e^{itH_w} + i\int_0^t dt' e^{i(t-t')H_w}Ve^{it'H_w}\right] \\ &= e^{-itH_w}e^{-\beta H_v}e^{itH_w} - e^{-itH_w}\int_0^\beta d\tau e^{-(\beta-\tau)H_v}Ve^{-\tau H_v}e^{itH_w} - i\int_0^t dt' e^{-i(t-t')H_w}Ve^{-it'H_w}e^{-\beta H_v}e^{itH_w} \\ &+e^{-itH_w}e^{-\beta H_v}i\int_0^t dt' e^{i(t-t')H_w}Ve^{it'H_w}+...\end{aligned}$$

Remark 1 *the normalized one must be divided by Partition function $Z(\beta)$*

consider the spatial representation

$$\begin{aligned}&\rho(\bar{x}'',t,\beta|\bar{x}') \\ &= \langle\bar{x}''|e^{-itH_w}e^{-\beta H_v}e^{itH_w}|\bar{x}'\rangle - \int_0^\beta d\tau\int d\bar{x}\langle\bar{x}''|e^{-itH_w}e^{-(\beta-\tau)H_v}|\bar{x}\rangle V(\bar{x})\langle\bar{x}|e^{-\tau H_v}e^{itH_w}|\bar{x}'\rangle \\ &-i\int_0^t dt'\int d\bar{x}\langle\bar{x}''|e^{-i(t-t')H_w}|\bar{x}\rangle V(\bar{x})\langle\bar{x}|e^{-it'H_w}e^{-\beta H_v}e^{itH_w}|\bar{x}'\rangle \\ &+i\int_0^t dt'\int d\bar{x}\langle\bar{x}''|e^{-itH_w}e^{-\beta H_v}e^{i(t-t')H_w}|\bar{x}\rangle V(\bar{x})\langle\bar{x}|e^{it'H_w}|\bar{x}'\rangle+... \\ &= \rho_\circ(\bar{x}'',t,\beta|\bar{x}') - \int_0^\beta d\tau\int d\bar{x}K_{\frac{1}{2}}(\bar{x}'',t,i(\beta-\tau)|\bar{x})V(\bar{x})K^*_{\frac{1}{2}}(\bar{x}',t,i\tau|\bar{x}) \\ &-i\int_0^t dt'\int d\bar{x}K_w(\bar{x}'',(t-t')|\bar{x})V(\bar{x})\rho_\circ(\bar{x},t',\beta|\bar{x}')+i\int_0^t dt'\int d\bar{x}\rho_\circ(\bar{x}'',(t-t'),\beta|\bar{x})V(\bar{x})K^*_w(\bar{x}',t\end{aligned}$$

because we are confused with the argument of the DM above so we leave it open for a while.

$$\rho\left(\bar{x}'', t, \beta|\bar{x}'\right) \equiv \rho_{\circ}\left(\bar{x}'', t, \beta|x'\right) + \rho_1^{\beta} + \rho_1^{t} + \rho_1^{t^{\star}}$$

I think the correct argument can be determined after we have done the explicit calculations.

the terms we need to re-calculate

$\langle\bar{x}|e^{it'H_w}|\bar{x}'\rangle, \langle\bar{x}''|e^{-i\left(t-t'\right)H_w}|\bar{x}\rangle$ these are simple harmonic Propagators

$\langle\bar{x}''|e^{-itH_w}e^{-(\beta-\tau)H_v}|\bar{x}\rangle, \langle\bar{x}|e^{-\tau H_v}e^{itH_w}|\bar{x}'\rangle$ these are something like intermediat propagators. or half density matrix

$\langle\bar{x}|e^{-it'H_w}e^{-\beta H_v}e^{itH_w}|\bar{x}'\rangle, \langle\bar{x}''|e^{-itH_w}e^{-\beta H_v}e^{i\left(t-t'\right)H_w}|\bar{x}\rangle$ we already has this one but the argument must be modified a little.

for the terms

$\langle\bar{x}|e^{-it'H_w}e^{-\beta H_v}e^{itH_w}|\bar{x}'\rangle = \int d\bar{y}\int d\bar{z}\langle\bar{x}|e^{-it'H_w}|\bar{y}\rangle\langle\bar{y}|e^{-\beta H_v}|\bar{z}\rangle\langle\bar{z}|e^{itH_w}|\bar{x}'\rangle$

$= \int d\bar{y}\int d\bar{z}K_w\left(\bar{x}, t'|\bar{y}\right)\rho_v\left(\bar{y}, \beta|\bar{z}\right)K_w^{*}\left(\bar{x}', t|\bar{z}\right)$

$\langle\bar{x}''|e^{-itH_w}e^{-\beta H_v}e^{i\left(t-t'\right)H_w}|\bar{x}\rangle = \int d\bar{y}\int d\bar{z}\langle\bar{x}''|e^{-itH_w}|\bar{y}\rangle\langle\bar{y}|e^{-\beta H_v}|\bar{z}\rangle\langle\bar{z}|e^{i\left(t-t'\right)H_w}|\bar{x}\rangle$

$= \int d\bar{y}\int d\bar{z}K_w\left(\bar{x}'', t'|\bar{y}\right)\rho_v\left(\bar{y}, \beta|\bar{z}\right)K_w^{*}\left(\bar{x}, (t-t')\,|\bar{z}\right)$

because the variables of time are not the same everwhere like in the previous case. To be sure we have to do the calculation again.

1.3.3 First perturbation term for distinguishable particles

we are trying to see the behaviour of the perturbation terms, so we start from the easiest term.

$$\tilde{\rho}^{(1)}\left(\bar{x}, \beta, t|\bar{x}\right) = \int_0^t dt'\int d\bar{x}\langle\bar{x}''|e^{-i\left(t-t'\right)H_w}|\bar{x}\rangle V\left(\bar{x}\right)\langle\bar{x}|e^{-it'H_w}e^{-\beta H_v}e^{itH_w}|\bar{x}'\rangle \tag{18}$$

We are interested in 2-particles interaction

$$V\left(\bar{x}\right) = \sum_{i\neq j}^{N} V\left(x_i - x_j\right) = \int dyV\left(y\right)\sum_{i\neq j}^{N}\delta\left(y - \left(x_i - x_j\right)\right)$$

$$= \int dyV\left(y\right)\sum_{i\neq j}^{N}\int\frac{dq}{2\pi}e^{-iqy}e^{iq\left(x_i - x_j\right)}$$

then the 1st correction term of density matrix is

$\tilde{\rho}^{(1)}\left(\bar{x}, \beta, t|\bar{x}\right) = \sum_{i\neq j}^{N}\int_0^t dt'\int\frac{dq}{2\pi}\int dyV\left(y\right)e^{-iqy}\int d\bar{x}'\langle\bar{x}''|e^{-i\left(t-t'\right)H_w}|\bar{x}'\rangle e^{iq\left(x_i' - x_j'\right)}\langle\bar{x}'|e^{-it'H_w}e^{-\beta H_v}e^{i}$

The Fourier transform of the density (non-normalized)

$$n_q^{(1)}(t) = \frac{1}{N}\sum_{\alpha=1}^{N}\int d\bar{x}\ \tilde{\rho}^{(1)}\left(\bar{x}, \beta, t|\bar{x}\right)e^{iqx_\alpha} \tag{19}$$

$= \frac{1}{N}\sum_{\alpha=1}^{N}\sum_{i\neq j}^{N}\int_0^t dt'\int\frac{dk}{2\pi}\int dyV\left(y\right)e^{-iky}\int d\bar{x}\int d\bar{x}'\langle\bar{x}|e^{-i\left(t-t'\right)H_w}|\bar{x}'\rangle e^{ik\left(x_i' - x_j'\right)}\langle\bar{x}'|e^{-it'H_w}e^{-\beta H_v}e^{itH_w}$

consider the term

$$C_3(q,k|t,t') \equiv \frac{1}{N}\sum_{\alpha=1}^{N}\sum_{i\neq j}^{N}\int d\bar{x}\int d\bar{x}'\langle\bar{x}|e^{-i(t-t')H_w}|\bar{x}'\rangle e^{ik\left(x_i'-x_j'\right)}\langle\bar{x}'|e^{-it'H_w}e^{-\beta H_v}e^{itH_w}|\bar{x}\rangle e^{iqx_\alpha}$$

$$= \frac{1}{N}\sum_{\alpha=1}^{N}\sum_{i\neq j}^{N}\int d\bar{x}\int d\bar{x}' K_w\left(\bar{x},(t-t')\,|\bar{x}'\right)e^{ik\left(x_i'-x_j'\right)}\rho_{w,v}^{(\beta)}\left(\bar{x}',t'-t|\bar{x}\right)e^{iqx_\alpha}$$

where

$K_w(x,(t-t')\,|x')$ is a simple harmonic oscillator propagator in real time

$\rho_{w,v}^{(\beta)}(x',t'-t|x)$ is a unequal-time density matrix of harmonic oscillator

$$\rho_{w,v}^{(\beta)}(x',t'-t|x) = \left(\frac{vw^2}{2\pi}\right)^{\frac{1}{2}}\left(\frac{1}{(w^2\cos wt'\cos wt+v^2\sin wt'\sin wt)\sinh v\beta - v\,wi\cosh v\beta\sin w(t-t')}\right)^{\frac{1}{2}}$$

$$\times\exp\left[\frac{w}{2}\left[\frac{i\sinh v\beta\left(w^2\cos wt\sin wt'+v^2\cos wt'\sin wt\right)-vw\cosh v\beta\cos w(t'-t)}{[(w^2\cos wt'\cos wt+v^2\sin wt'\sin wt)\sinh v\beta - vwi\cosh v\beta\sin w(t-t')]}\right]x^2\right]$$

$$\times\exp\left[-\frac{w}{2}\left[\frac{i\sinh v\beta\left(v^2\cos wt\sin wt'+w^2\sin wt\cos wt'\right)+wv\cosh v\beta\cos w\left(t'-t\right)}{(w^2\cos wt'\cos wt+v^2\sin wt'\sin wt)\sinh v\beta - v\,wi\cosh v\beta\sin w(t-t')}\right](x')^2\right]$$

$$\times\exp\left[-\frac{w}{2}\frac{-2wvxx'}{[(w^2\cos wt'\cos wt+v^2\sin wt'\sin wt)\sinh v\beta - vwi\cosh v\beta\sin w(t-t')]}\right]$$

note that this $\rho_{w,v}^{(\beta)}(x',t'-t|x)$ is a more general case of the previous result (the zeroth order). One can see easily by setting $t'=t$ this expression will reduce to the zeroth order DM.

And we can see by this general expression for different time that the system which is Time-translation invariant was broken the symmetry when the diffent value of trap frequency is switched on.110

1.3.4 Three-point Correlation function for distinguishable particles

$$C_3(q,k|t,t') = \frac{1}{N}\sum_{\alpha=1}^{N}\sum_{i\neq j}^{N}\int d\bar{x}\int d\bar{x}' K_w\left(\bar{x},(t-t')\,|\bar{x}'\right)e^{ik\left(x_i'-x_j'\right)}\rho_{w,v}^{(\beta)}\left(\bar{x}',t'-t|\bar{x}\right)e^{iqx_\alpha} \tag{20}$$

there are 3 possiblities of the *triple sum* $\sum_{\alpha,i,j}$

1. $\alpha = i$;

$$\frac{1}{N}\sum_{i\neq j}^{N}\int d\bar{x}\int d\bar{x}' K_w\left(\bar{x},(t-t')\,|\bar{x}'\right)e^{ik\left(x_i'-x_j'\right)}\rho_{w,v}^{(\beta)}\left(\bar{x}',t'-t|\bar{x}\right)e^{iqx_i}$$

$$= \frac{1}{N}\sum_{i}^{N}\sum_{j}^{N}\int d\bar{x}\int d\bar{x}' K_w\left(\bar{x},(t-t')\,|\bar{x}'\right)e^{ik\left(x_i'-x_j'\right)}\rho_{w,v}^{(\beta)}\left(\bar{x}',t'-t|\bar{x}\right)e^{iqx_i}$$

$$-\frac{1}{N}N^2\int d\bar{x}e^{iqx_i}\int d\bar{x}' K_w\left(\bar{x},(t-t')\,|\bar{x}'\right)\rho_{w,v}^{(\beta)}\left(\bar{x}',t'-t|\bar{x}\right)$$

$$= \frac{1}{N}\sum_{i}^{N}\sum_{j}^{N}\int d\bar{x}e^{iqx_i}\int d\bar{x}' K_w\left(\bar{x},(t-t')\,|\bar{x}'\right)e^{ik\left(x_i'-x_j'\right)}\rho_{w,v}^{(\beta)}\left(\bar{x}',t'-t|\bar{x}\right)$$

$$-N\int d\bar{x}\rho_o\left(\bar{x},t,\beta|\bar{x}\right)e^{iqx_i}$$ see Dirac notation,is this last term simply $n_q^{(0)}(t)$?so is it going to dive

consider the term

$$\int d\bar{x}e^{iqx_i}\int d\bar{x}' K_w\left(\bar{x},(t-t')\,|\bar{x}'\right)e^{ik\left(x_i'-x_j'\right)}\rho_{w,v}^{(\beta)}\left(\bar{x}',t'-t|\bar{x}\right)$$

$$= \int d\bar{x}e^{iqx_i}\left[\prod_{l=1\neq i,j}^{N}\int dx_l' K_w\left(x_l,(t-t')\,|x_l'\right)\rho_{w,v}^{(\beta)}\left(x_l',t'-t|x_l\right)\right]$$

$\times \left[\int dx_i' K_w\left(x_i,(t-t')\left|x_i'\right.\right) e^{ikx_i'} \rho_{w,v}^{(\beta)}\left(x_i', t'-t|x_i\right)\right] \left[\int dx_j' K_w\left(x_j,(t-t')\left|x_j'\right.\right) e^{-ikx_j'} \rho_{w,v}^{(\beta)}\left(x_j', t'-t|\right.\right.$

We doubt that the last 2 terms in square brackets have the same results but different only the indices, anyway we are going to evaluate it explicitly.

2. $\alpha = j$;

$\frac{1}{N} \sum_{i \neq j}^{N} \int d\bar{x} \int d\bar{x}' K_w\left(\bar{x},(t-t')\left|\bar{x}'\right.\right) e^{ik\left(x_i'-x_j'\right)} \rho_{w,v}^{(\beta)}\left(\bar{x}', t'-t|\bar{x}\right) e^{iqx_j}$

3. $\alpha \neq i \neq j$;

$\frac{1}{N} \sum_{\alpha=1}^{N-2} \sum_{i \neq j}^{N} \int d\bar{x} \int d\bar{x}' K_w\left(\bar{x},(t-t')\left|\bar{x}'\right.\right) e^{ik\left(x_i'-x_j'\right)} \rho_{w,v}^{(\beta)}\left(\bar{x}', t'-t|\bar{x}\right) e^{iqx_\alpha}$

Before we proceed further, the perturbation expansion has to be justified.

Conclusion 2 *In this work we have calculated the quasi-static excitation (beathing mode) of the Bose Eistein Condensation of Boson gas in a spherical magnetic trap by the method of many-body path integrals. We found that the non-interacting model gives the perpetual oscillation of the condensate while in the experiment the damping of the oscillation was found. It is generally accepted that the damping is due to the interaction between bosons. However, when we attemps to include the intraction into the calculation together with statistics, we found that the three-points correlation function is needed and it is too tedious to calculate this quantity.*

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BOSON PAIRING IN 2D T-J MODEL FOR TRIANGULAR LATTICE

KOBCHAI TAYANASANTI TO PROF.V.A. IVANOV AND PROF. J.T.DEVREESE.

ABSTRACT. Replace this text with your own abstract.

1. CRITICAL TEMPERATURE FOR BOSON PAIRING IN 2D TRIANGULAR LATTICE

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2. INTRODUCTION

The 2-fermions condensation of Cooper pairing is well known in Superconductivity but in the boson case there occur only 1-boson condensation (BEC). Historically, some pioneer works had been done unsuccesfully for the possibility of boson pairing. However, the important developtment was done by M.J.Rice and Y.R.Wang [3]. They shown that the 2-particles boson pairing is possible in 2 dimensional system. They also claimed that their results have a possible implication of the interpretation of the superconductivity in perovskite oxides and of the order parameter in 2D liquid He^4 layers. Recently, in the work by M.Yu. Kagan and D.V. Efremov[2], have shown the possible symmetries of boson pairing in 2D square lattice based on t-J model. However, they found that the Phase seperation occurs earlier than the bosons pairing in the case of one band and one type of bosons.

The motivation of this work is to investigate the possibility of Bosons pairing in two dimensional triangular lattice. The model used for the system is 2D t-J model. The aim of this work is to find the phase diagram between particle density n versus the interaction strength $\frac{J}{t}$. From this diagram we can see the region where the pairing with different kinds of symmetry occur until the Phase Seperation happen. We proceed this work by following the method by M.Yu Kagan and T.M. Rice[1] and some results from the work of Ivanov et.al.[4]. We will proceed the work by calculate the critical temperature for pairing to see which kind of symmetries are possible. Then the threshold for pairing can be found in order to construct the $n - \frac{J}{t}$phase diagram. (Howeve, we still do not know how to find the boundary of phase seperation or threshold value of $\frac{J}{t}$ that cause the phase seperation occurs.)

3. Theoretical Model

We follow the work by M.Yu. Kagan and D.V. Efremov, the systen is described by the Hamiltonian,

$$H = -t\sum_{ij} b_i^\dagger b_j + \frac{U}{2}\sum_j n_i^2 - V\sum_{ij} n_i n_j \tag{3.1}$$

Making Fourier Transform we obtain,

$$H = \sum_{\vec{p}} \epsilon_{\vec{p}} b_{\vec{p}}^\dagger b_{\vec{p}} + \frac{U}{2}\sum_{\vec{k}\ \vec{k}'\vec{q}} b_{\vec{k}}^\dagger b_{\vec{k}'}^\dagger b_{\vec{k}'-\vec{q}} b_{\vec{k}+\vec{q}} - 2\sum_{\vec{k}\ \vec{k}'\vec{q}} V(\vec{q})\, b_{\vec{k}}^\dagger b_{\vec{k}+\vec{q}} b_{\vec{k}'}^\dagger b_{\vec{k}'-\vec{q}} \tag{3.2}$$

where in the case of Triangular lattice
$\vec{q} = \vec{p} - \vec{p}'$ (2D vector)
$\varepsilon_{\vec{p}} = -2t\left(\cos P_y + 2\cos\frac{P_y}{2}\cos\frac{\sqrt{3}P_x}{2}\right)$,
$V(\vec{q}) = V\left(\cos q_y + 2\cos\frac{q_y}{2}\cos\frac{\sqrt{3}q_x}{2}\right)$
(For the geometry of the lattice, see [4])

4. Possible Symmetries Consideration

Now we can consider the possible symmetries of pairing from the gap equation in momentum representation.

$$\Delta(\vec{p}) = \sum_{p'} \frac{V(\vec{p}-\vec{p}')\Delta(\vec{p}')}{2\sqrt{(\varepsilon_p-\mu)^2+\Delta^2(\vec{p}')}} \coth\left[\frac{\sqrt{(\varepsilon_p-\mu)^2+\Delta^2(\vec{p}')}}{2T}\right] \tag{4.1}$$

where
$\Delta(\vec{p})$ is an order parameter or energy gap
μ is a chemical potential
To find the critical temperature T_c, we can neglect the 2^{nd} order term of $\Delta(\vec{p})$ because as $T \longrightarrow T_c$ the oreder parameter $\Delta \longrightarrow 0$.The order parameter and the potential can be expanded in basis set of functions $\{\eta_i(\vec{p})\}, i = 1,2,..,6$ for Triangular lattice. Then we can write

$$\Delta(\vec{p}) = \sum_{i=1}^{6} \Delta_i \eta_i(\vec{p}) \tag{4.2}$$

$$V(\vec{p}-\vec{p}') = 2V\sum_{i=1}^{6} \eta_i(\vec{p})\,\eta_i(\vec{p}') \tag{4.3}$$

where[4]

$$
\begin{aligned}
\eta_1(\vec{p}) &= \frac{1}{\sqrt{3}}\left(\cos P_y + 2\cos\frac{P_y}{2}\cos\frac{\sqrt{3}P_x}{2}\right) \\
\eta_2(\vec{p}) &= \frac{2}{\sqrt{6}}\left(\cos P_y - 2\cos\frac{P_y}{2}\cos\frac{\sqrt{3}P_x}{2}\right) \\
\eta_3(\vec{p}) &= \sqrt{2}\sin\frac{P_y}{2}\sin\frac{\sqrt{3}P_x}{2} \\
\eta_4(\vec{p}) &= \frac{1}{\sqrt{3}}\left(\sin P_y + 2\cos\frac{P_y}{2}\cos\frac{\sqrt{3}P_x}{2}\right) \\
\eta_5(\vec{p}) &= \frac{2}{\sqrt{6}}\left(\sin P_y - \cos\frac{P_y}{2}\cos\frac{\sqrt{3}P_x}{2}\right) \\
\eta_6(\vec{p}) &= \sqrt{2}\cos\frac{P_y}{2}\sin\frac{\sqrt{3}P_x}{2}
\end{aligned} \tag{4.4}
$$

The basis functions describe different symmetry. For singlet $\eta_1(\vec{p})$ is for s-pairing, $\eta_2(\vec{p})$ is for $d_{x^2-y^2}$ pairing, $\eta_3(\vec{p})$ is for d_{xy} pairing, and $\eta_{4,5,6}(\vec{p})$ are linear combination of basis function for the triplet-pairing.

Substitute these 2 equations into the gap equation

$$\sum_{i=1}^{6}\Delta_i\eta_i(\vec{p}) = 2V\sum_{p'}\frac{1}{2(\varepsilon_p-\mu)}\coth\left[\frac{(\varepsilon_p-\mu)}{2T_c}\right]\left(\sum_{i=1}^{6}\Delta_i\eta_i(\vec{p})\right)\left(2V\sum_{j=1}^{6}\eta_j(\vec{p})\eta_j(\vec{p}')\right)$$

Multiply both sides by $\eta_k(\vec{p})$ and integrate over momentum. By using the fact that $\int\int\frac{dP_x dP_y}{(2\pi)^2}\eta_i(\vec{p})\eta_j(\vec{p}) = \delta_{ij}$ we have

$$\Delta_k = 2V\sum_{p'}\sum_{i=1}^{6}\frac{\Delta_i}{2\sqrt{\varepsilon_p-\mu}}\eta_k(\vec{p}')\eta_j(\vec{p}')\coth\left[\frac{\sqrt{\varepsilon_p-\mu}}{2T_c}\right] \tag{4.5}$$

Solving for T_c ,we have the secular equation

$$\det\left|\delta_{ij} - 2V\sum_{\vec{p}}\frac{\coth\frac{(\varepsilon_p-\mu)}{2T_c}}{2(\varepsilon_p-\mu)}\eta_i(\vec{p})\eta_j(\vec{p})\right| = 0 \tag{4.6}$$

One can show easily that many terms in the above matrix vanish because when we change $\sum_{\vec{p}} \longrightarrow \int\int\frac{dP_x dP_y}{(2\pi)^2}$ most of the matrix elements vanish beacause of the odd functions of the integrands. Only the terms involving $\eta_1(\vec{p})\eta_1(\vec{p})$,$\eta_1(\vec{p})\eta_2(\vec{p})$, $\eta_2(\vec{p})\eta_1(\vec{p})$,and $\eta_2(\vec{p})\eta_2(\vec{p})$ are survived. Which coresponding to the $s^* + d_{x^2-y^2}$ and d_{xy} pairing symmetry. (Actually other diagonal element such as $\eta_3(\vec{p})\eta_3(\vec{p})$,... are non vanishing too but they are too small so we will not consider here).

5. Critical Temperature for Pairing

To find the critical temperature of the occurence of bosons pairing we start from gap equation for bosons at $T < T_c$. Expanding the Gap function or order parameter in the basis of symmetry group C_3 gives a secular equation4.6

$$\det\left|\delta_{ij} - 2V\sum_{\vec{p}} \frac{\coth\frac{(\varepsilon_p-\mu)}{2T_c}}{2(\varepsilon_p-\mu)}\eta_i(\vec{p})\eta_j(\vec{p})\right| = 0 \tag{5.1}$$

Due to the complexity of the exact expressions, let consider first in the small momentum regime$\vec{p} \longrightarrow 0$

$\eta_1(\vec{p}) \approx \frac{1}{\sqrt{3}}\left(5 - \frac{3\vec{P}^2}{4}\right)$; $\vec{P}^2 = P_y^2 + P_x^2$

$\eta_2(\vec{p}) \approx -\frac{2}{\sqrt{6}}\left(1 + \frac{3}{8}\vec{P}^2\cos 2\phi\right)$

$\eta_3(\vec{p}) \approx \frac{1}{4}\sqrt{\frac{3}{2}}\vec{P}^2\sin 2\phi$

$\phi = \arctan\frac{P_x}{P_y}$ (note that this is uncommon definition because we follow the orientation of the lattice defined in [4]).

for the kinetic energy

$\varepsilon_{\vec{p}} \approx -10t + \frac{\vec{P}^2}{2m}$; $m \equiv \frac{1}{3t}$ =boson mass for the Triangular lattice case.then

$(\varepsilon_p - \mu) \equiv \frac{\vec{P}^2}{2m} - \mu'$; $\mu' \equiv 10t + \mu$

The value of the Chemical potential μ', is always negative and can be determined from the particles number conservation constraint.

$$n_B = \int\int \frac{d^2p}{(2\pi)^2}\left[\exp\left(\frac{\frac{\vec{P}^2}{2m} - \mu'}{T}\right) - 1\right]^{-1} \tag{5.2}$$

solving this equation gives

$$\mu' = -T\exp\left(-\frac{1}{T}\frac{2\pi n_B}{m}\right) \tag{5.3}$$

From the above secular equation, change sum to integral over momentum and firsly consider the case of d_{xy} which the secular equation is not a matrix.

$$1 = \sqrt{3}\frac{2V}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\frac{\pi}{\sqrt{3}}}^{\frac{\pi}{\sqrt{3}}} dP_x dP_y \frac{\coth\frac{\left(\frac{\vec{P}^2}{2m} + |\mu'|\right)}{2T_c}}{2\left(\frac{\vec{P}^2}{2m} + |\mu'|\right)}\eta_3(\vec{p})\eta_3(\vec{p})$$

because of the unsymmetry of the limit of integration of P_x and P_y So I propose to simplify by approximation

$$\int_{-\pi}^{\pi}\int_{-\frac{\pi}{\sqrt{3}}}^{\frac{\pi}{\sqrt{3}}} dP_x dP_y \longrightarrow \int_0^{2\pi} d\phi \int_0^{\frac{2\pi}{\sqrt{3}}} PdP$$

(this point need more discussions since I don't know if it could make any effects to symmetry). Hence

$$1 = \frac{3\sqrt{3}m^3V}{2\pi}T_c^2\int_0^{\frac{4\pi^2}{12mT_c}} \frac{\coth\left(x + \frac{|\mu'|}{2T_c}\right)}{\left(x + \frac{|\mu'|}{2T_c}|\right)}x^2dx$$

and because we are interested to find T_c so by using the relation

$$\mu'|_{T=T_c} = -T_c \exp\left(-\frac{1}{T_c}\frac{2\pi n_B}{m}\right)$$

substitute in to the secular equation gives

$$1 = \frac{3\sqrt{3}m^2V}{2\pi}T_c^2\int_0^{\frac{4\pi^2}{12mT_c}} \frac{\coth\left(x+\frac{1}{2}\exp\left(-\frac{1}{T_c}\frac{2\pi n_B}{m}\right)\right)}{\left(x+\frac{1|}{2}\exp\left(-\frac{1}{T_c}\frac{2\pi n_B}{m}\right)\right)}x^2dx \tag{5.4}$$

which can be solve self consistently numerically whenever we know values of all parameters.

For another kind of symmetry $s^* + d_{x^2-y^2}$ we have to solve the secular equation

$$\begin{vmatrix} 1-\sqrt{3}\frac{2V}{(2\pi)^2}\int d^2P\frac{\coth\frac{\left(\frac{\vec{p}^2}{2m}+|\mu'|\right)}{2T_c}}{2\left(\frac{\vec{p}^2}{2m}+|\mu'|\right)}\eta_1(\vec{p})\eta_1(\vec{p}) & -\sqrt{3}\frac{2V}{(2\pi)^2}\int d^2P\frac{\coth\frac{\left(\frac{\vec{p}^2}{2m}+|\mu'|\right)}{2T_c}}{2\left(\frac{\vec{p}^2}{2m}+|\mu'|\right)}\eta_1(\vec{p})\eta_2(\vec{p}) \\ -\sqrt{3}\frac{2V}{(2\pi)^2}\int d^2P\frac{\coth\frac{\left(\frac{\vec{p}^2}{2m}+|\mu'|\right)}{2T_c}}{2\left(\frac{\vec{p}^2}{2m}+|\mu'|\right)}\eta_1(\vec{p})\eta_2(\vec{p}) & 1-\sqrt{3}\frac{2V}{(2\pi)^2}\int d^2P\frac{\coth\frac{\left(\frac{\vec{p}^2}{2m}+|\mu'|\right)}{2T_c}}{2\left(\frac{\vec{p}^2}{2m}+|\mu'|\right)}\eta_2(\vec{p})\eta_2(\vec{p}) \end{vmatrix} = 0$$

From analysis of the work by M.Yu. Kagan and D.V.Efremov[2], they claimed that the integral of the type

$$\int pdp\frac{\coth\frac{\xi}{2T}}{2\xi}p^4 \longrightarrow 0 \quad \text{as } p \longrightarrow 0$$

we can see easily by changing variable $p^2 = \varepsilon \longrightarrow 0$ then the integral reads
$\sim \int d\varepsilon\frac{\coth\varepsilon}{\varepsilon}\varepsilon^2 \sim \int d\varepsilon\frac{1}{\varepsilon^2}\varepsilon^2 = \varepsilon \longrightarrow 0$
and another type is

$$\int pdp\frac{\coth\frac{\xi}{2T}}{2\xi}p^2 \sim \int d\varepsilon\frac{\coth\varepsilon}{\varepsilon}\varepsilon \sim \int d\varepsilon\frac{1}{\varepsilon} = \ln\varepsilon$$

Hence we conclude that there is no critical temperature for the pairing of these types. Consider in the case of $s^* + d_{x^2-y^2}$,

$\eta_1(\vec{p})\eta_1(\vec{p}) = \frac{1}{3}\left(25 + \frac{9\vec{P}^4}{16} - \frac{15\vec{P}^2}{4}\right)$

$\eta_1(\vec{p})\eta_2(\vec{p}) = -\frac{2}{3\sqrt{2}}\left(5 - \frac{3\vec{P}^2}{4} + \frac{15}{8}\vec{P}^2\cos 2\phi - \frac{9}{32}\vec{P}^4\cos 2\phi\right)$

$\eta_2(\vec{p})\eta_2(\vec{p}) = \frac{2}{3}\left(1 + \frac{3}{4}\vec{P}^2\cos 2\phi + \frac{9}{64}\vec{P}^4\cos^2 2\phi\right)$

if we neclect all the terms involving $\vec{P}^2$ and $\vec{P}^4$ then

$$1 - 9I + \frac{148}{9}I^2 = 0$$

where $I = \sqrt{3}\frac{2V}{(2\pi)^2}\int d^2P\frac{\coth\frac{\left(\frac{\vec{p}^2}{2m}+|\mu'|\right)}{2T_c}}{2\left(\frac{\vec{p}^2}{2m}+|\mu'|\right)} = \frac{\sqrt{3}V}{2\pi}m\int_0^{\frac{\pi^2}{3mT_c}}\frac{\coth\left(x+\frac{1}{2}\exp\left(-\frac{1}{T_c}\frac{2\pi n_B}{m}\right)\right)}{\left(x+\frac{1}{2}\exp\left(-\frac{1}{T_c}\frac{2\pi n_B}{m}\right)\right)}dx$

Substitute this expression into the secular equation above then we can find the T_c of the boson pairing with $s^* + d_{x^2-y^2}$ symmetry.

By the way, if $\frac{|\mu'|}{2T_c} \ll 1$, we can do the integral analytically, i.e.

$$\int_0^{\frac{\pi^2}{3mT_c}} \frac{\coth\left(x+\frac{1}{2}\exp\left(-\frac{1}{T_c}\frac{2\pi n_B}{m}\right)\right)}{\left(x+\frac{1}{2}\exp\left(-\frac{1}{T_c}\frac{2\pi n_B}{m}\right)\right)}dx \approx \int_0^{\frac{\pi^2}{3mT_c}} \frac{1}{\left(x+\frac{1}{2}\exp\left(-\frac{1}{T_c}\frac{2\pi n_B}{m}\right)\right)^2}dx$$
$$= \frac{4\pi^2 e^{\frac{4}{T_c}\pi\frac{n_B}{m}}}{2\pi^2 e^{\frac{2}{T_c}\pi\frac{n_B}{m}}+3mT_c} \approx \frac{|\mu'|}{2T_c}$$

then the secular equation above is

$$1-9\left(\frac{\sqrt{3}V}{2\pi}m\frac{\exp\left(-\frac{1}{T_c}\frac{2\pi n_B}{m}\right)}{2}\right)+\frac{148}{9}\frac{\sqrt{3}V}{2\pi}m\left(\frac{\sqrt{3}V}{2\pi}m\frac{\exp\left(-\frac{1}{T_c}\frac{2\pi n_B}{m}\right)}{2}\right)^2=0$$

Solution are :

$$T_c^{\pm} = \frac{\frac{2\pi n_B}{m}}{\left(\ln\frac{37V^2m^2}{27\pi^2}\left(1\pm\sqrt{\left(1-\frac{296\sqrt{3}\pi}{729}Vm\right)}\right)^{-1}\right)}$$
$$= \frac{T_\circ}{\left(\ln\frac{37}{4*27\pi^2}\frac{V^2}{t^2}\left(1\pm\sqrt{\left(1-\frac{296\sqrt{3}\pi}{2*729}\frac{V}{t}\right)}\right)^{-1}\right)}$$

The higher value of T_c is considered as a physical one. and $T_\circ$ is the degenracy temperature $T_\circ = \frac{2\pi n_B}{m}$.

6. Threshold for Boson Pairing

To construct the phase diagram, we need to know the critical value of $\frac{J}{t}$ that cause the 2-particles bound state. We can determine the bound state by looking at the value of the T-matrix for two particles in vacuum with zero momentum(i.e. the two bosons have momentum $\vec{p}$ and $-\vec{p}$). From the last section we know already that the only possible pairing is $s^* + d_{x^2-y^2}$ so we shall concentrate on this symmetry. The T-matrix can be found by firstly solving the Bethe-Salpeter equation and consider it in the case of low momentum$\left(T_{s^*+d_{x^2-y^2}}(E) = \lim_{pp'\to 0} T_{\vec{p}\vec{p}'}(E)\right)$. In the case of t-J model, U is a strong hard core repulsive which we will take limit to infinity later. The basis function of the $s^* + d_{x^2-y^2}$ symmetry is

$$\varphi(\vec{p}) \equiv \eta_1(\vec{p}) + \eta_2(\vec{p}) = \left(\frac{1+\sqrt{2}}{\sqrt{3}}\right)\cos P_y + \left(\frac{2-\sqrt{2}}{\sqrt{3}}\right)\cos\frac{P_y}{2}\cos\frac{\sqrt{3}P_x}{2} \tag{6.1}$$

And the Lippmann-Schwinger equation for T-matrix reads,

$$T_{\vec{p}\vec{p}'}(E) = V_{\vec{p}\vec{p}'} + \int\int \frac{dp_x''dp_x''}{(2\pi)^2}\frac{V_{\vec{p}\vec{p}''}T_{\vec{p}''\vec{p}'}(E)}{E+4t\left(\cos P_y + 2\cos\frac{P_y}{2}\cos\frac{\sqrt{3}P_x}{2}\right)} \tag{6.2}$$

we can expand the function (see also [5])

$$T_{\vec{p}\vec{p}'}(E) = T_1(E) + T_2(E)\left(\varphi(\vec{p})+\varphi(\vec{p}')\right) + T_3(E)\varphi(\vec{p})\varphi(\vec{p}') \tag{6.3}$$

and

$$V_{\vec{p}\vec{p}'} = U - 2V\varphi(\vec{p})\varphi(\vec{p}')$$

Substitute these into ?? and comparing the coefficient of the basis functions we arrive at the algebraic euations of $T_{1,2,3}(E)$

$$\begin{aligned} T_1 &= U + UT_1 I_\circ + UT_2 I_x \\ T_2 &= -J(T_1 I_x + T_2 I_{xx}) \\ T_3 &= -J(1 + T_3 I_{xx} + T_2 I_x) \end{aligned} \tag{6.4}$$

where

$$\begin{aligned} I_\circ &= \int\int \frac{dp_x dp_y}{(2\pi)^2} \frac{1}{E + 4t\left(\cos P_y + 2\cos\frac{P_y}{2}\cos\frac{\sqrt{3}P_x}{2}\right)} \\ I_x &= \int\int \frac{dp_x dp_y}{(2\pi)^2} \frac{\left[\left(\frac{1+\sqrt{2}}{\sqrt{3}}\right)\cos P_y + \left(\frac{2-\sqrt{2}}{\sqrt{3}}\right)\cos\frac{P_y}{2}\cos\frac{\sqrt{3}P_x}{2}\right]}{E + 4t\left(\cos P_y + 2\cos\frac{P_y}{2}\cos\frac{\sqrt{3}P_x}{2}\right)} \\ I_{xx} &= \int\int \frac{dp_x dp_y}{(2\pi)^2} \frac{\left[\left(\frac{1+\sqrt{2}}{\sqrt{3}}\right)\cos P_y + \left(\frac{2-\sqrt{2}}{\sqrt{3}}\right)\cos\frac{P_y}{2}\cos\frac{\sqrt{3}P_x}{2}\right]^2}{E + 4t\left(\cos P_y + 2\cos\frac{P_y}{2}\cos\frac{\sqrt{3}P_x}{2}\right)} \end{aligned}$$

6.0.1. *Low momentum approximation.* The energy reads
$E + 4t\left(\cos P_y + 2\cos\frac{P_y}{2}\cos\frac{\sqrt{3}P_x}{2}\right) \sim$
$E + 4t\left(\left(1 - \frac{1}{2}P_y^2\right) + 2\left(1 - \frac{1}{8}P_y^2\right)\left(1 - \frac{3}{8}P_x^2\right)\right) = 12t + E - 3tP_x^2 - 3tP_y^2 + \ldots$
neglect the term of 4th order.
The fisrt integral $I_\circ$.

$$\begin{aligned} I_\circ &= \int\int \frac{dp_x dp_y}{(2\pi)^2} \frac{1}{12t + E - 3tP_x^2 - 3tP_y^2} \\ &= \frac{1}{(2\pi)^2}\int_{-\frac{\pi}{\sqrt{3}}}^{\frac{\pi}{\sqrt{3}}} dp_x \int_{-\pi}^{\pi} dp_y \frac{1}{12t + E - 3tP_x^2 - 3tP_y^2} \\ &= \frac{1}{(2\pi)^2}\int_{-\frac{\pi}{\sqrt{3}}}^{\frac{\pi}{\sqrt{3}}} dx \int_{-\pi}^{\pi} dy \frac{1}{12t + E - 3t(x^2 + y^2)} \\ &\sim \frac{1}{(2\pi)^2}\int_{-\frac{\pi}{\sqrt{3}}}^{\frac{\pi}{\sqrt{3}}} dx \int_{-\pi}^{\pi} dy \frac{1}{12t + E - 3t(x^2 + y^2)} \\ &= \frac{1}{6\pi t}\int_0^{\pi} \frac{r}{4 + \frac{E}{3t} - r^2} dr \\ &= \frac{1}{6\pi t}\ln\left(\frac{E + 12t}{E + 12t - 3\pi^2 t}\right) \end{aligned}$$

Note the we make approximation of the limit of integration $\frac{\pi}{\sqrt{3}} \to \pi$ to make the polar integration possible.

second Integral I_x. $\varphi(\vec{p}) = \left(\frac{1+\sqrt{2}}{\sqrt{3}}\right)\cos P_y + \left(\frac{2-\sqrt{2}}{\sqrt{3}}\right)\cos\frac{P_y}{2}\cos\frac{\sqrt{3}P_x}{2}$

$$\begin{aligned}
&\sim \left(\tfrac{1+\sqrt{2}}{\sqrt{3}}\right)\left(1-\tfrac{1}{2}P_y^2\right)+\left(\tfrac{2-\sqrt{2}}{\sqrt{3}}\right)\left(1-\tfrac{1}{8}P_y^2\right)\left(1-\tfrac{3}{8}P_x^2\right)\\
&=\sqrt{3}\left(1-\tfrac{1}{4}P_x^2+\tfrac{1}{8}P_x^2\sqrt{2}-\tfrac{1}{8}P_y^2\sqrt{2}-\tfrac{1}{4}P_y^2\right)\\
&=\sqrt{3}\left(1-\tfrac{1}{4}\left(1-\tfrac{\sqrt{2}}{2}1\right)P_x^2-\tfrac{1}{4}\left(1+\tfrac{\sqrt{2}}{2}\right)P_y^2\right)
\end{aligned}$$

$$\begin{aligned}
I_x &= \int\int \frac{dp_x dp_y}{(2\pi)^2}\frac{\left(\frac{1+\sqrt{2}}{\sqrt{3}}\right)\cos P_y+\left(\frac{2-\sqrt{2}}{\sqrt{3}}\right)\cos\frac{P_y}{2}\cos\frac{\sqrt{3}P_x}{2}}{E+4t\left(\cos P_y+2\cos\frac{P_y}{2}\cos\frac{\sqrt{3}P_x}{2}\right)}\\
&= \sqrt{3}\int\int\frac{dp_x dp_y}{(2\pi)^2}\frac{\left(1-\frac{1}{4}\left(1-\frac{\sqrt{2}}{2}\right)P_x^2-\frac{1}{4}\left(1+\frac{\sqrt{2}}{2}\right)P_y^2\right)}{12t+E-3tP_x^2-3tP_y^2}\\
&= \sqrt{3}\left(I_\circ-\frac{1}{4}\left(1-\frac{\sqrt{2}}{2}\right)I_2-\frac{1}{4}\left(1+\frac{\sqrt{2}}{2}\right)I_1\right)
\end{aligned}$$

where

$$\begin{aligned}
I_1 &= \int\int\frac{dp_x dp_y}{(2\pi)^2}\frac{P_y^2}{12t+E-3tP_x^2-3tP_y^2}\\
I_2 &= \int\int\frac{dp_x dp_y}{(2\pi)^2}\frac{P_x^2}{12t+E-3tP_x^2-3tP_y^2}
\end{aligned}$$

consider each integral seperately.

$$\begin{aligned}
I_1 &= \int\int\frac{dp_x dp_y}{(2\pi)^2}\frac{P_y^2}{12t+E-3tP_x^2-6tP_y^2}\\
&= \frac{1}{(2\pi)^2}\int_{-\frac{\pi}{\sqrt{3}}}^{\frac{\pi}{\sqrt{3}}}dp_x\int_{-\pi}^{\pi}dp_y\frac{P_y^2}{12t+E-3tP_x^2-3tP_y^2}\\
&\sim \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}dx\int_{-\pi}^{\pi}dy\frac{y^2}{12t+E-3t\left(x^2+y^2\right)}\\
&= \frac{1}{3t\left(2\pi\right)^2}\int_0^{\pi}\frac{r^3}{4+\frac{E}{3t}-r^2}dr\int_0^{2\pi}\sin^2\theta d\theta\\
&= \frac{1}{12\pi t}\int_0^{\pi}\frac{r^3}{4+\frac{E}{3t}-r^2}dr\\
&= \frac{1}{72\pi t^2}\left(-3\pi^2 t+(E+12t)\ln\frac{(E+12t)}{(E+12t-3\pi^2 t)}\right)=I_2
\end{aligned}$$

Let define in the same fashion of [1]

$$\begin{aligned}
\tilde{E} &\equiv E+12t\\
\Omega &= \ln\frac{(E+12t)}{(E+12t-3\pi^2 t)}=\ln\frac{\tilde{E}}{\tilde{E}-3\pi^2 t}
\end{aligned}\tag{6.5}$$

then

$$
\begin{aligned}
I_\circ &= \frac{1}{6\pi t}\Omega \\
I_1 &= I_2 = \frac{1}{72\pi t^2}\left(-3\pi^2 t + \tilde{E}\Omega\right)
\end{aligned} \tag{6.6}
$$

So now we can evaluate I_x

$$
\begin{aligned}
I_x &= \sqrt{3}\left(I_\circ - \frac{1}{4}\left(1-\frac{\sqrt{2}}{2}\right)I_1 - \frac{1}{4}\left(1+\frac{\sqrt{2}}{2}\right)I_1\right) \\
&= \sqrt{3}\left(I_\circ - \frac{1}{2}I_1\right) \\
&= \sqrt{3}\left(\frac{1}{6\pi t}\Omega - \frac{1}{144\pi t^2}\left(-3\pi^2 t + \tilde{E}\Omega\right)\right)
\end{aligned} \tag{6.7}
$$

For the integral I_{xx}, the factor of $\varphi(\vec{p})^2$ can be approximate to

$\varphi^2(\vec{p}) = \left(\left(\frac{1+\sqrt{2}}{\sqrt{3}}\right)\cos P_y + \left(\frac{2-\sqrt{2}}{\sqrt{3}}\right)\cos\frac{P_y}{2}\cos\frac{\sqrt{3}P_x}{2}\right)^2$

$\sim 3\left(1-\frac{1}{4}\left(1-\frac{\sqrt{2}}{2}1\right)P_x^2 - \frac{1}{4}\left(1+\frac{\sqrt{2}}{2}\right)P_y^2\right)^2$

$= 3\left(1+\frac{1}{2}\left(\frac{\sqrt{2}}{2}-1\right)P_x^2 - \frac{1}{2}\left(1+\frac{\sqrt{2}}{2}\right)P_y^2\right)$

then

$$
\begin{aligned}
I_{xx} &= \int\int \frac{dp_x dp_y}{(2\pi)^2} \frac{\left[\left(\frac{1+\sqrt{2}}{\sqrt{3}}\right)\cos P_y + \left(\frac{2-\sqrt{2}}{\sqrt{3}}\right)\cos\frac{P_y}{2}\cos\frac{\sqrt{3}P_x}{2}\right]^2}{E + 4t\left(\cos P_y + 2\cos\frac{P_y}{2}\cos\frac{\sqrt{3}P_x}{2}\right)} \\
&\approx 3\int\int \frac{dp_x dp_y}{(2\pi)^2} \frac{\left(1+\frac{1}{2}\left(\frac{\sqrt{2}}{2}-1\right)P_x^2 - \frac{1}{2}\left(1+\frac{\sqrt{2}}{2}\right)P_y^2\right)}{12t + E - 3tP_x^2 - 3tP_y^2} \\
&= 3\left(I_\circ + \frac{1}{2}\left(\frac{\sqrt{2}}{2}-1\right)I_1 - \frac{1}{2}\left(1+\frac{\sqrt{2}}{2}\right)I_1\right) \\
&= 3\left(I_\circ - I_1\right) = 3\left(\frac{1}{6\pi t}\Omega - \frac{1}{72\pi t^2}\left(-3\pi^2 t + \tilde{E}\Omega\right)\right)
\end{aligned}
$$

Summary 1.

$$
\begin{aligned}
I_\circ &= \frac{1}{6\pi t}\Omega \\
I_x &= \sqrt{3}\left(\frac{1}{6\pi t}\Omega - \frac{1}{144\pi t^2}\left(-3\pi^2 t + \tilde{E}\Omega\right)\right) \\
I_{xx} &= 3\left(\frac{1}{6\pi t}\Omega - \frac{1}{72\pi t^2}\left(-3\pi^2 t + \tilde{E}\Omega\right)\right)
\end{aligned} \tag{6.8}
$$

The Solutions of 6.4 are [1]

$$
\begin{aligned}
T_1 &= \frac{U\left(1+JI_{xx}\right)}{\left(1-UI_\circ\right)\left(1+JI_{xx}\right)+UJI_x^2} \\
T_2 &= \frac{-UJI_x}{\left(1-UI_\circ\right)\left(1+JI_{xx}\right)+UJI_x^2} \\
T_3 &= \frac{-J\left(1-UI_\circ\right)}{\left(1-UI_\circ\right)\left(1+JI_{xx}\right)+UJI_x^2}
\end{aligned} \tag{6.9}
$$

For $U \to \infty$ then

$$
\begin{aligned}
T_1 &= \frac{\left(1+JI_{xx}\right)}{\left(-I_\circ\right)\left(1+JI_{xx}\right)+JI_x^2} \\
T_2 &= \frac{-JI_x}{\left(-I_\circ\right)\left(1+JI_{xx}\right)+JI_x^2} \\
T_3 &= \frac{JI_\circ}{\left(-I_\circ\right)\left(1+JI_{xx}\right)+JI_x^2}
\end{aligned} \tag{6.10}
$$

Now we can solve the T-matrix problem for $s^* + d_{x^2-y^2}$ pairing, consider the vertex function at small momentum limit

$$
\begin{aligned}
T_{s^*+d_{x^2-y^2}}(E) &= \lim_{pp'\to 0} T_{\vec{p}\vec{p}'}(E) \\
&= \lim_{pp'\to 0}\left[T_1(E)+T_2(E)\left(\varphi(\vec{p})+\varphi(\vec{p}')\right)+T_3(E)\varphi(\vec{p})\varphi(\vec{p}')\right] \\
&= T_1(E)+2\sqrt{3}T_2(E)+3T_3(E)
\end{aligned} \tag{6.11}
$$

Then using the equations 6.10, we have

$$
T_{s^*+d_{x^2-y^2}}(E) = \frac{1+3JI_\circ-2\sqrt{3}JI_x+JI_{xx}}{\left(-I_\circ\right)\left(1+JI_{xx}\right)+JI_x^2}
$$

Then we can fill in by 6.8

$$
\begin{aligned}
I_\circ &= \frac{1}{6\pi t}\Omega \\
I_x &= \sqrt{3}\left(\frac{1}{6\pi t}\Omega-\frac{1}{144\pi t^2}\left(-3\pi^2 t+\tilde{E}\Omega\right)\right) \\
I_{xx} &= 3\left(\frac{1}{6\pi t}\Omega-\frac{1}{72\pi t^2}\left(-3\pi^2 t+\tilde{E}\Omega\right)\right)
\end{aligned} \tag{6.12}
$$

$$
\begin{aligned}
T(E) &= \frac{1+3J\frac{1}{6\pi t}\Omega-6J\left(\frac{1}{6\pi t}\Omega-\frac{1}{144\pi t^2}\left(-3\pi^2 t+\tilde{E}\Omega\right)\right)+3J\left(\frac{1}{6\pi t}\Omega-\frac{1}{72\pi t^2}\left(-3\pi^2 t+\tilde{E}\Omega\right)\right)}{\left(-\frac{1}{6\pi t}\Omega\right)\left(1+J3\left(\frac{1}{6\pi t}\Omega-\frac{1}{72\pi t^2}\left(-3\pi^2 t+\tilde{E}\Omega\right)\right)\right)+3J\left(\frac{1}{6\pi t}\Omega-\frac{1}{144\pi t^2}\left(-3\pi^2 t+\tilde{E}\Omega\right)\right)} \\
&= \frac{1}{-\frac{1}{6\pi t}\Omega+\frac{J}{t^2}\left(\frac{1}{768}\pi^2-\frac{1}{1152}\frac{\tilde{E}}{t}\Omega\left(1+\frac{1}{6\pi^2}\frac{\tilde{E}}{t}\Omega\right)\right)}
\end{aligned} \tag{6.13}
$$

We consider in the case of small binding energy $\tilde{E} = E + 12t \sim 0$ which means the begining of pairing. This means that the terms dependent on $\tilde{E}$ can be neglect. Hence the T-matrix becomes,

$$T_{s^*+d_{x^2-y^2}}(E) = \frac{1}{\frac{1}{768}\pi^2\frac{J}{t^2} - \frac{1}{6\pi t}\Omega} \tag{6.14}$$

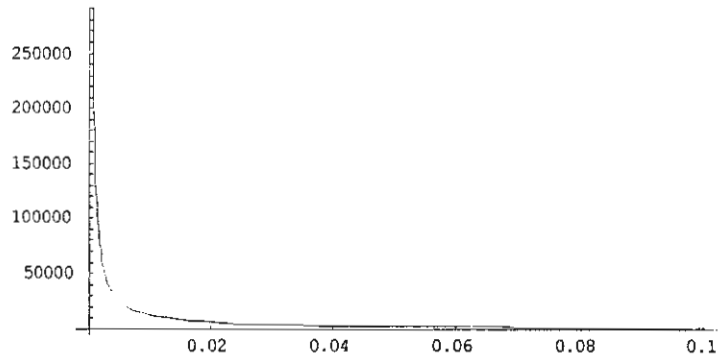
6.1. **Bound state consideration.** From the T-matrix 6.14 we can see that, for $\frac{J}{t} < \frac{128}{\pi^3}\Omega = \frac{128}{\pi^3}\ln\frac{\tilde{E}}{\tilde{E}-3\pi^2 t}$, the T-matrix is negative which means the two particles bound state occurs and we can evealuate for the bound state energy

$$|\tilde{E}| = \frac{\pi^2 W}{4\left(1-\exp\left(-\frac{\pi^3}{128}\frac{J}{t}\right)\right)} \tag{6.15}$$

where $W = 12t$ the bandwidth of the triangular lattice.
We can consider the relationship

$$\frac{|\tilde{E}|}{t} = \frac{3\pi^2}{1-\exp\left(-\frac{\pi^3}{128}\frac{J}{t}\right)}$$

which can be shown in the picture



where the vertical axe is $\frac{|\tilde{E}|}{t}$ and the horizon one is $\frac{J}{t}$. However, this result must be justified more.

6.2. **The Critical Temperature of Pairing from Bethe-Salpeter equation.** We have already calculated the critical temperature of $s^* + d_{x^2-y^2}$ pairing by considering from the order parameter or gap equation. Here, by knowing the expression for the T-matrix6.14 we can calculate the critical temperature by another way. By this method we can know the anlytical expression of the temperature which depends on the binding energy. Consider the Bethe-salpeter equation,

$$\Gamma_{s^*+d_{x^2-y^2}} = \frac{T_{s^*+d_{x^2-y^2}}\left(\tilde{E}\right)}{1+T_{s^*+d_{x^2-y^2}}\left(\tilde{E}\right)\int\int\frac{dp_x dp_y}{(2\pi)^2}\frac{\coth\frac{\varepsilon_{\vec{p}}-\mu}{2T}}{2\left(\varepsilon_{\vec{p}}-\mu\right)}} \tag{6.16}$$

$\varepsilon_{\vec{p}} = -2t\left(\left(1-\frac{1}{2}P_y^2\right)+2\left(1-\frac{1}{8}P_y^2\right)\left(1-\frac{3}{8}P_x^2\right)\right) = -6t+\frac{3}{2}tP_x^2+\frac{3}{2}tP_y^2+\ldots$
$\varepsilon_{\vec{p}} \approx -6t+\frac{\vec{P}^2}{2m}$, and $m=\frac{1}{3t}$.
and we absorb $-6t$ to μ by redefine the chemical potential $\tilde{\mu} = \mu + 6t$. The T-matrix which enter in Bethe-Salperter equation have to be evaluated at the binding

energy $\tilde{E} = 2\tilde{\mu}$. and $\tilde{\mu}$ can be determined from the equation for conservation of the number of particles.

$$n = \int\int \frac{dp_x dp_y}{(2\pi)^2} \frac{1}{\exp\left(\frac{\frac{p^2}{2m} - \tilde{\mu}}{2T}\right) - 1} \tag{6.17}$$

which can be solved easily and we use the same crude approximation as in the previous section, we arrive at the solution

$$\tilde{\mu} = -T \exp\left(-\frac{1}{T}\frac{2\pi n_B}{m}\right)$$

And the Temperature can be found from the pole of 6.16

$$1 + T_{s^*+d_{x^2-y^2}}\left(\tilde{E}\right) \int\int \frac{dp_x dp_y}{(2\pi)^2} \frac{\coth\frac{\varepsilon_{\vec{p}}-\mu}{2T}}{2\left(\varepsilon_{\vec{p}} - \mu\right)} = 0 \tag{6.18}$$

which we can use the same calculation procedure as done in the previous section.

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PATH INTEGRAL APPROACH TO A SINGLE POLYMER CHAIN WITH EXCLUDED VOLUME EFFECT

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The effect of a polymer chain with excluded volume representing the long-range interaction between segments along the chain is studied using the Feynman path integral method. The main problem is to calculate the mean square distance, $< R^2 >$, that is

$$< R^2 >= AN^{\nu}$$

where N is the degree of polymerization, ν is a scaling exponent varying from 1-2 for free chain and stiff chain, respectively; and A is a coefficient that depends on the details of the polymer. In the case that the excluded volume interactions are present, $\nu = 6/5$.

The model proposed by Edwards and Singh [1] and Muthukumar and Nickel [2] are employed. Instead of using the idea of an effective step-length technique and the perturbation technique, the idea of Feynman [3] in relation to the polaron problem is used and developed by handling a disordered system. The idea is to model the polymer action as a model of quardatic trial action and consider the differences between the polymer action and the trial action as the first cumulant approximation in one parameter. The variational principle is used to find the optimal values of the variational parameters and the mean square distance is obtained. A comparison between these approaches and effective step-length and perturbation approach will be discussed.

1 Introduction

The theory of the excluded volume effect in a polymer chain is one of the central problems in the field of polymer solution theory representing the effect of the interaction between segments which are far apart along the chain. This interaction is often called the long-range interaction in contrast to the short-range interaction representing the interaction among a few neighbouring segments.

The polymer excluded volume problem is of the same form and difficulty as the general many body problem, first discussed by Kuhn [4]. The modern development was initiated by Flory [5]. It is recognized that the long-range interaction changes the statistical property of the chain entirely.

The main problem is to calculate the mean square end-to-end distance $\langle R^2 \rangle$, that is

$$< R^2 >= AN^{\nu} \tag{1.1}$$

where the exponent $1<\nu<2$, is to be determined and appears to be solely a function of the dimensionality of space.

Over past decades many attempts have endeavoured to understand the excluded volume effect. One of the theories of the polymer excluded volume problem is the Edwards and Singh's method. A simple method capable of adoption in more complicated problems is developed using the idea of an effective step-length. The mean square value of R^2 is developed as a series which for large L is

$$R^2 = \omega^{\frac{2}{5}} L^{\frac{6}{5}} l^{\frac{2}{5}} (1.12 + 1.05 + 1.03 + ...) \qquad (1.2)$$

where length $L = Nl$ and ω is the self repulsion.

Another theory is the perturbation which represents a simple derivation of the mean square end-to-end distance $\langle R^2 \rangle$ of a linear-flexible chain as a perturbation series in the dimensionless excluded volume parameter z_d. In an essential way the method used Laplace transforms with respect to the contour length L. The results, to orders six and four in space dimension $d = 3$ and 2, respectively, are

$$\langle R^2 \rangle = Ll[1 + \frac{4}{3} z_3 - 2.075385396\, z_3^2 + 6.296879676\, z_3^3 - 25.05725072\, z_3^4 + 116.134785\, z_3^5 - 594.71663\, z_3^6 + ...], \; d = 3,$$

$$\langle R^2 \rangle = Ll[1 + \frac{1}{2} z_2 - 0.12154525\, z_2^2 + 0.02663136\, z_2^3 - 0.13223603\, z_2^4 + ...], \; d = 2.$$

The purpose of this paper is to calculate the mean square end-to-end distance, employing the model proposed by Edwards [6] and using the idea of Feynman in the polaron problem and one developed by us for handling disordered systems [7]. The idea is to model the system with a trial action containing adjustable, to be determined, parameters. Once the trial action is introduced, the average distribution G can be calculated by expanding in first cumulant approximation about the corresponding trial average distribution G_0. G, approximated by the first cumulant, G_1 can be obtained.

As mentioned above, the parameters should be determined by minimizing the exponent of G_1. However, this procedure leads to a complication because the parameters will depend parametrically on the initial and final position of the polymer chain. To avoid such a complication, a simpler approximation in which only the diagonal contribution of the exponent of G_1 is used in the minimization. This approximation is equivalent to minimizing the free energy. Once the

parameters are obtained they will be used to calculate the mean square end-to-end distance.

The outline of the paper is as follows: section 2 is a brief review of an effective step-length technique and the perturbation technique. In section 3, Edwards' model is reviewed. The path integral approach with one parameter model is introduced in section 4. In section 5, the results are discussed and compared with other presentations. Finally, in order to be able to carry out the calculations arising in section 4, an appendix gives a detailed derivation of a characteristic functional corresponding to the trial action $S_0(\omega)$.

2 The Mean Square Distance

2.1 *The Effective Step Length Technique*

The excluded volume problem is a central part of polymer solution theory, the mean-square end-to-end distance agreed on $\langle R^2 \rangle \propto L^{\alpha}$ where $\alpha = 6/5$ is shown to within one to two percent. Analytic theories based on self consistent fields give α to be exactly 6/5. The chain is considered a locus in space *r(s)*, *s* the arc length, and the random walk constraint is represented by the Wiener measure

$$\exp[-\frac{3}{2l}\int \dot{r}^2(s)ds] \tag{2.1.1}$$

and the interaction

$$\exp\{-\omega\int_0^L\int_0^L \delta[r(s)-r(s')]dsds'\}. \tag{2.1.2}$$

This allows the consideration of $\omega > 0$. The step-length is l, and ω has the dimensions of volume. If the symbol $(D(r))$ denotes integration over all paths, then

$$\langle R^2 \rangle = \frac{\int_{r(0)=0}^{r(L)=R} D(r)[r(L)-r(0)]^2 \exp(A)}{\int d^3R \int_{r(0)=0}^{r(L)=R} \exp(A)D(r)} . \tag{2.1.3}$$

Instead it can argued that an effective step-length l_1 be introduced, so that, by definition

$$\langle R^2 \rangle = Ll_1 . \tag{2.1.4}$$

Therefore one can write

$$\frac{3}{2l}\int \dot{r}^2 ds + \omega \iint D[r(s) - r(s')] ds ds'$$

$$= \frac{3}{2l_1}\int \dot{r}^2 ds + \{\frac{3}{2}(\frac{1}{l} - \frac{1}{l_1})\int \dot{r}^2 ds + \omega \iint D[r(s) - r(s')] ds ds'\} \tag{2.1.5}$$

$$= \frac{3}{2l_1}\int \dot{r}^2 ds + B \text{ , say} \tag{2.1.6}$$

$$= C + B. \tag{2.1.7}$$

Then

$$\langle R^2 \rangle = Ll_1 + O(B) + O(B^2) + O(B^3) + \ldots \tag{2.1.8}$$

At this point, choose l_1 so that

$$\langle R^2 \rangle = Ll_1$$

so that to first order in B, it gives the equation

$$Ll_1^2(\frac{1}{l} - \frac{1}{l_1}) = 2\sqrt{\frac{6}{\pi^3}}\omega \frac{L^{\frac{3}{2}}}{l_1^{\frac{1}{2}}}. \tag{2.1.9}$$

The solution to this equation clearly subsumes perturbation theory, for if ω is small, $l \cong l_1$,

$$\langle R^2 \rangle = Ll + 2\sqrt{\frac{6}{\pi^3}}\omega L^{\frac{3}{2}} l^{\frac{-1}{2}}. \tag{2.1.10}$$

But for $L^{\frac{1}{2}} > \omega$ there is a Flory type equation with solution

$$l_1 = (2)^{\frac{2}{5}}(\frac{6}{\pi^3})^{\frac{1}{5}}\omega^{\frac{2}{5}} l^{\frac{2}{5}} L^{\frac{6}{5}} \tag{2.1.11}$$

so that

$$\langle R^2 \rangle = (2)^{\frac{2}{5}}(\frac{6}{\pi^3})^{\frac{1}{5}}\omega^{\frac{2}{5}} l^{\frac{2}{5}} L^{\frac{6}{5}}. \tag{2.1.12}$$

To establish the stability of the index α against higher approximations, $\langle R^2 \rangle$ can be written as follows

$$\langle R^2 \rangle = Ll + \frac{A\omega L^{\frac{3}{2}}}{l^{\frac{1}{2}}} + \frac{B\omega^2 L^2}{l^2} + \frac{C\omega^3 L^{\frac{5}{2}}}{l^{\frac{7}{2}}} \qquad (2.1.13)$$

where A, B, and C are numbers. Now effective step length l can be introduced to give

$$l = l_1[1 - l_1(\frac{1}{l} - \frac{1}{l_1}) + l_1^2(\frac{1}{l} - \frac{1}{l_1})^2 ...] \qquad (2.1.14)$$

Using equation (2.1.14) in (2.1.13) it get to the third in ω

$$\langle R^2 \rangle = Ll_1 - Ll_1^2(\frac{1}{l} - \frac{1}{l_1}) + Ll_1^3(\frac{1}{l} - \frac{1}{l_1})^2 + \frac{A\omega L^{\frac{3}{2}}}{l_1^{\frac{1}{2}}} + \frac{A\omega L^{\frac{3}{2}}}{2} l_1^{\frac{1}{2}}(\frac{1}{l} - \frac{1}{l_1})$$

$$+ \frac{B\omega^2 L^2}{l_1^2} + 2B\omega^2 \frac{l^2}{l_1}(\frac{1}{l} - \frac{1}{l_1}) + \frac{C\omega^3 L^{\frac{5}{2}}}{l^{\frac{7}{2}}} - \qquad (2.1.15)$$

Thus the first order approximation gives

$$\alpha = 1.059\omega^{\frac{1}{5}} L^{\frac{1}{10}} l^{\frac{-3}{10}} \qquad (2.1.16)$$

$$\langle R^2 \rangle \sim \alpha^2 \sim Ll_1 = 1.12\omega^{\frac{2}{5}} L^{\frac{6}{5}} l^{\frac{2}{5}}.$$

Now to the second order contained is

$$\alpha = 1.025\omega^{\frac{1}{5}} L^{\frac{1}{10}} l^{\frac{-3}{10}} \qquad (2.1.17)$$

$\langle R^2 \rangle$ still retains the form $\sim \omega^{\frac{2}{5}} L^{\frac{1}{10}} l^{\frac{-3}{10}}$. Now to the third order where

$$\alpha = 1.015\omega^{\frac{1}{5}} L^{\frac{1}{10}} l^{\frac{-3}{10}},$$

$$\langle R^2 \rangle \sim \alpha^2 = 1.03\omega^{\frac{2}{5}} L^{\frac{6}{5}} l^{\frac{2}{5}}. \qquad (2.1.18)$$

Finally this can be expressed in a series for $\langle R^2 \rangle$, the additions coming from the order of expansion

$$\langle R^2 \rangle = \omega^{\frac{2}{5}} L^{\frac{6}{5}} l^{\frac{2}{5}} (1.12 + 1.05 + 1.03 + ...). \qquad (2.1.19)$$

2.2 The Perturbation Technique

The net effect of the excluded volume interaction between segments of the polymer chain is usually repulsive and leads to an expansion of the chain size. When the excluded volume interaction is very weak, a perturbation theory for the ratio of the mean square end-to-end distance is $\langle R^2 \rangle$ of the chain. Its unperturbed value $\langle R^2 \rangle_0$ can be developed and reduced to a varies in a single dimensionless interaction parameter z_d [8] as

$$\frac{\langle R^2 \rangle}{\langle R^2 \rangle_0} = 1 + C_1 z_d + C_2 z_d^2 + C_3 z_d^3 + ... \qquad (2.2.1)$$

In describing the approach to equation (2.2.1) the equation starts directly with the continuum model and works entirely with the Laplace transform functions $\tilde{G}(E) = \int_0^{\infty} G(L) e^{-EL} dL$, where G(L) are probability functions for a chain's contour length L.

For the standard discrete Gaussian chain model of N+1 segments, the probability distribution function $G_0(R,n)$ can be evaluated and a term of the contour length $L = N l$ is given by

$$G_0(R,L) = \left(\frac{d}{2\pi L l}\right)^{d/2} \exp\left(-\frac{dR^2}{2Ll}\right) . \qquad (2.2.2)$$

The mean square end-to-end distance of the Gaussian chain is

$$\langle R^2 \rangle_0 = \int d^d R R^2 G_0(R,L) \Big/ \int d^d R G_0(R,L)$$
$$= Ll. \qquad (2.2.3)$$

When interactions are introduced, the bare distribution will be modified to a non-Gaussian $G(R,L)$ with corresponding characteristic function $\hat{G}(k,L)$ and propagator $\tilde{G}(k,E_0)$. The mean square end-to-end chain distance is given by

$$\langle R^2 \rangle = \int d^d R R^2 G(R,L) \Big/ \int d^d R G(R,L)$$

$$= l \frac{\int \frac{dE_0}{2\pi i} e^{E_0 L} [-\frac{2d}{l} \frac{\partial}{\partial k^2} \tilde{G}(k, E_0)]_{k=0}}{\int \frac{dE_0}{2\pi i} e^{E_0 L} \tilde{G}(0, E_0)} \quad . \quad (2.2.4)$$

This can define a new variable, The so-call "renormalized" energy E by

$$E \equiv E_0 + \Sigma(0, E_0) \quad . \quad (2.2.5)$$

This definition can be reverted order-by-order in perturbation theory to yield $E_0(E)$. If this is defined as

$$\tilde{\Sigma}(k, E) \equiv \tilde{\Sigma}[k, E_0(E)] \quad , \quad (2.2.6)$$

then the exact propagator becomes

$$\tilde{G}[k, E_0(E)] = \frac{1}{E + \frac{k^2 l}{2d} + \tilde{\Sigma}(k, E) - \tilde{\Sigma}(0, E)} \quad . \quad (2.2.7)$$

These results can be expressed as functions of E and the equation (2.2.4) rewritten as

$$\langle R^2 \rangle = l \int \frac{dE}{2\pi i} e^{EL} F_{2(E)} \Big/ \int \frac{dE}{2\pi i} e^{EL} F_1(E) \quad , \quad (2.2.8)$$

where

$$F_1(E) = E^{-1} J \exp[(E_0 - E)L],$$
$$F_2(E) = E^{-1} K F_1(E) L], \quad (2.2.9)$$

where

$$J = \frac{dE_0}{dE} = 1 - \frac{d}{dE} \tilde{\Sigma}(0, E),$$
$$K = 1 + \frac{2d}{l} \frac{\partial}{\partial k^2} \tilde{\Sigma}(k, E) |_{k=0} \quad . \quad (2.2.10)$$

Solving these simultaneous equations in (2.2.9) for F_1 and F_2 , d = 3 is obtained and

$$\langle R^2 \rangle = Ll[1 + \sum_{m=1} C_m z_3^m] \ , \tag{2.2.11}$$

where the coefficients through order m = 6 are

$$z_3 \equiv (\frac{3}{2\pi})^{3/2} \frac{\omega L^{1/2}}{l^{3/2}}, C_1 = 4/3, C_2 = \frac{28\pi}{27} - \frac{16}{3}, C_3 \approx 6.296879676 \ ,$$
$$C_4 \approx -25.05725072 \ , C_5 \approx 116.134785 \ , C_6 \approx -594.71663 \ . \tag{2.2.12}$$

For d = 2, the calculation of $\langle R^2 \rangle$ runs in an exactly analogous manner to the above derivation in d = 3. Then

$$\langle R^2 \rangle = Ll[1 + \sum_{m=1} C_m z_2^m] \tag{2.2.13}$$

where

$$z_2 \equiv \frac{\omega L}{\pi l}, C_1 = 1/2, C_2 = -0.1215452 \ ,$$
$$C_3 = 0.0266313 \ , C_4 = -0.13223603 \ . \tag{2.2.14}$$

3 Edwards' Model

In an ideal polymer, there is only a short-range interaction and the action can be written as

$$S = \frac{3}{2l^2} \int_0^N d\tau \dot{R}^2(\tau) \tag{3.1}$$

where l is the effective bond length representing the short-range interaction, and $R(\tau)$ is the position of segment τ of the polymer.

Since there are many effects in real polymers, the long-range interaction is quite complicated: steric effects, Van der Waals attraction, and solvent molecules effect. However, for the large-length scale concerned, the details of the interaction can be omitted. Thus the interaction between the polymer segments τ and σ can be expressed as

$$k_B T v(R_\tau - R_\sigma) \ .$$

This can be approximated even further by a delta function

$$v k_B T \delta(R_\tau - R_\sigma) \ ,$$

where v is the excluded volume which represents the long-range interaction, and has the dimension of volume.

The total interaction energy is thus written as

$$U_1 = \frac{v}{2} k_B T \int_0^N \int_0^N d\tau d\sigma \delta(R(\tau) - R(\sigma)) \tag{3.2}$$

using the local concentration of the segments

$$c(r) = \int_0^N d\tau \delta(r - R(\tau)) \ . \tag{3.3}$$

Thus, equation (3.2) may be rewritten

$$U_1 = \int d\, r \frac{1}{2} v k_B T c(r)^2 \ . \tag{3.4}$$

This statement indicates that equation (3.2) is the first term in the virial expansion of the free energy with respect to the local concentration $c(r)$. Now if the interaction equation (3.2) is taken into account, the action becomes

$$S = \frac{3}{2l^2} \int_0^N d\tau \dot{R}^2(\tau) + \frac{v}{2} \int_0^N \int_0^N d\tau d\sigma \delta(R(\tau) - R(\sigma)) \ . \tag{3.5}$$

The second term accounts for excluded volume interactions between segments of the polymer. The probability distribution of the end-to-end distance is given by

$$G(R_2, R_1; N) = \int_{R_1}^{R_2} D[R(\tau)] e^{-S} \ . \tag{3.6}$$

4 Path Integral Approach

In this section, we apply the idea of Feynman, developed for the polaron problem, and Sa-yakanit[9], applied to disorder system, to polymer problem . This idea is to model the system with a model trial action which can be solved exactly for one parameter model.

The Edwards action is exactly solvable only in the limit, v = 0, where no excluded volume interactions are presented. In this case, the polymer exhibits Gaussian statistics. If v is not zero, the model is no longer exactly solvable;

However, this problem is similar to a polaron problem, which can be solved by path integral and variation method, by introducing the trial action $S_0(\omega)$.

$$S_0(\omega)=\frac{m}{2}\int_0^N d\tau \dot{R}^2(\tau)+\frac{m\omega^2}{4N}\int_0^N\int_0^N d\tau d\sigma(R(\tau)-R(\sigma))^2 \qquad (4.1)$$

where $m = 3\hbar^2$ and ω is a parameter.

Once the trial action $S_0(\omega)$ has been introduced, it is possible to find the average distribution which, from equation (3.6) can be rewritten as

$$G(R_2,R_1;N)=G_0(R_2,R_1;N,\omega)<\exp[S_0(\omega)-S]>_{S_0(\omega)}, \qquad (4.2)$$

where the trial distribution $G_0(R_2,R_1;N,\omega)$ is defined by

$$G_0(R_2,R_1;N)=\int_{R_1}^{R_2} D[R(\tau)]e^{-S_0(\omega)}, \qquad (4.3)$$

and the average $<x>_{S_0(\omega)}$ is defined as

$$<X>_{S_0(\omega)}=\frac{\int_0^N D[R(\tau)]Xe^{-S_0(\omega)}}{\int_0^N D[R(\tau)]e^{-S_0(\omega)}} \qquad (4.4)$$

Approximating equation (4.2) by the first cumulant, we get

$$G_1(R_2,R_1;N)=G_0(R_2,R_1;N,\omega)<\exp[S_0(\omega)-S]>_{S_0(\omega)}. \qquad (4.5)$$

To obtain $G_1(R_2,R_1;N)$, find $G_0(R_2,R_1;N)$ and the average. Firstly, consider the average $<S_0(\omega)-S>_{S_0(\omega)}$. Since the first term in S and $S_0(\omega)$ always cancel each other, this denotes $<S>_{S_0(\omega)}$ and $<S_0(\omega)>_{S_0(\omega)}$ for convenience as the averages of the second term respectively. The average of $<S>_{S_0(\omega)}$ can be evaluated by making a Fourier decomposition of $\delta(R(\tau)-R(\sigma))$. Thus,

$$\langle S\rangle_{S_0(\omega)}=\frac{V}{2}\int_0^N\int_0^N d\tau d\sigma\left(\frac{1}{2\pi}\right)^3\int dk\left\langle\exp[ik.(R(\tau)-R(\sigma))]\right\rangle_{S_0(\omega)} \qquad (4.6)$$

The average on the right-hand side of equation (4.6) can be expanded in cumulants, and because $S_0(\omega)$ is quadratic, only the first two cumulants are non-zero [10]. Equation (4.6) becomes

$$\langle S\rangle_{S_0(\omega)} = \frac{V}{2}\int_0^N\int_0^N d\tau d\sigma\left(\frac{1}{2\pi}\right)^3 \int dk \exp(x_1 + x_2) \quad , \tag{4.7}$$

where

$$x_1 = ik.\langle R(\tau) - R(\sigma)\rangle_{S_0(\omega)} \quad , \tag{4.8}$$

and

$$x_2 = \frac{-k^2}{2}\left[\frac{1}{3}\left\langle (R(\tau) - R(\sigma))^2\right\rangle_{S_0(\omega)} - \langle R(\tau) - R(\sigma)\rangle_{S_0(\omega)}\right] \quad . \tag{4.9}$$

Note that the second term inside the square brackets of equation (4.9) represents only one component of the coordinates. Performing the k-integration results in

$$\langle S\rangle_{S_0(\omega)} = \frac{V}{2}\int_0^N\int_0^N d\tau d\sigma\left(\frac{1}{2\pi}\right)^3 A^{-3/2}\exp\left(\frac{-B^2}{4A}\right) \tag{4.10}$$

where

$$A = \frac{1}{2}\left[\frac{1}{3}\left\langle (R(\tau) - R(\sigma))^2\right\rangle_{S_0(\omega)} - \langle R(\tau) - R(\sigma)\rangle_{S_0(\omega)}\right] \tag{4.11}$$

and

$$B = i\langle R(\tau) - R(\sigma)\rangle_{S_0(\omega)} \quad . \tag{4.12}$$

Next we consider the average of $< S_0(\omega) >_{S_0(\omega)}$ which is easily written as

$$\langle S_0(\omega)\rangle_{S_0(\omega)} = \frac{m\omega^2}{4N}\int_0^N\int_0^N d\tau d\sigma\left\langle (R(\tau) - R(\sigma))^2\right\rangle_{S_0(\omega)} \quad . \tag{4.13}$$

4.1 The Characteristic Functional

From equations (4.10) and (4.13) it can be seen that the average $< S_0(\omega) - S >_{S_0(\omega)}$ can be expressed solely in terms of the following averages: $< R(\tau) >_{S_0(\omega)}$ and $< R(\tau)R(\sigma) >_{S_0(\omega)}$. Such averages can be obtained from a characteristic functional of

$< \exp(\int_0^N d\tau f(\tau)R(\tau)) >_{S_e(\omega)}$. From Feynman and Hibbs, the characteristic functional can be expressed as

$$< \exp(\int_0^N d\tau f(\tau)R(\tau)) >_{S_e(\omega)} = \exp\left(-\left[S'_{0,cl}(R_2 - R_1; N, \omega) - S_{0,cl}(R_2 - R_1; N, \omega)\right]\right) , \tag{4.1.1}$$

where $S'_{0,cl}(R_2 - R_1; N, \omega)$ and $S_{0,cl}(R_2 - R_1; N, \omega)$ are two classical actions which we have derived from the calculation in the Appendix. Once the classical action $S'_{0,cl}(R_2 - R_1; N, \omega)$ is obtained, we can differentiate expression (4.1.1) with respect to f(τ) to obtain

$$\begin{aligned}\langle R(\tau)\rangle_{S_e(\omega)} &= -\frac{\delta S'_{0,cl}(R_2 - R_1; N, \omega)}{\delta f(\tau)}\Big|_{f(\tau)=0} \\ &= \frac{m\omega}{2\sinh\omega N}\left[\frac{2R_2}{m\omega}\left(\sinh\omega\tau + 2\sinh\frac{\omega N}{2}\sinh\frac{\omega(N-\tau)}{2}\sinh\frac{\omega\tau}{2}\right)\right. \\ &\quad \left. + \frac{2R_1}{m\omega}\left(\sinh\omega(N-\tau) + 2\sinh\frac{\omega N}{2}\sinh\frac{\omega(N-\tau)}{2}\sinh\frac{\omega\tau}{2}\right)\right] \end{aligned} \tag{4.1.2}$$

where the symbol $|_{f(\tau)=0}$ implies that after the differentiation, f(τ)=0 must be set. Continuing the differentiation,

$$\begin{aligned}\langle R(\tau)R(\sigma)\rangle_{S_e(\omega)} = [&-\frac{\delta^2 S'_{0,cl}(R_2 - R_1; N, \omega)}{\delta f(\tau)\delta f(\sigma)} \\ &+ \frac{\delta S'_{0,cl}(R_2 - R_1; N, \omega)}{\delta f(\tau)} \cdot \frac{\delta S'_{0,cl}(R_2 - R_1; N, \omega)}{\delta f(\sigma)}]\,|_{f(\tau)=0} .\end{aligned} \tag{4.1.3}$$

Set σ = τ in equation(4.1.3) to obtain

$$\left\langle R^2(\tau)\right\rangle_{S_0(\omega)} = \frac{3}{m\omega}\left\{\frac{\sinh\omega(N-\tau)\sinh\omega\tau}{\sinh\omega N} + \frac{4\sinh^2\frac{\omega}{2}(N-\tau)\sinh^2\frac{\omega}{2}\tau}{\sinh\omega N}\right\}$$
$$+\left[R_2\left(\frac{\sinh\omega\tau}{\sinh\omega N} + \frac{2\sinh\frac{\omega N}{2}\sinh\frac{\omega(N-\tau)}{2}\sinh\frac{\omega\tau}{2}}{\sinh\omega N}\right)\right.$$
$$\left.+R_1\left(\frac{\sinh\omega(N-\tau)}{\sinh\omega N} + \frac{2\sinh\frac{\omega N}{2}\sinh\frac{\omega(N-\tau)}{2}\sinh\frac{\omega\tau}{2}}{\sinh\omega N}\right)\right]^2 . \tag{4.1.4}$$

Equation (4.1.4) is the mean square end-to-end distance of the polymer. This method is more general than another methods because the mean square can be found at any point along the polymer chain.

Using equations (4.1.2) and (4.1.3) and performing the integration in equation (4.13) the following is obtained:

$$\left\langle S_0(\omega)\right\rangle_{S_0(\omega)} = \frac{3}{2}\left(\frac{\omega N}{2}\coth\frac{\omega N}{2} - 1\right)$$
$$+\frac{m}{2}\left[\frac{\omega N}{2}\coth\frac{\omega N}{2} - \left(\frac{\omega N}{2}\operatorname{cosech}\frac{\omega N}{2}\right)^2\right]\frac{(R_2-R_1)^2}{2N} . \tag{4.1.5}$$

Collecting the above results, the following is obtained:

$$G_1(R_2-R_1;N,\omega) = \left(\frac{3}{2\pi N l^2}\right)^{3/2}\left(\frac{\omega N}{2\sinh\frac{\omega N}{2}}\right)^3$$
$$\exp\left[\left(\frac{-3\omega}{4l^2}\right)(R_2-R_1)^2\left(\frac{1}{2}\coth\frac{\omega N}{2} + \frac{\omega N}{4}\operatorname{cosech}^2\frac{\omega N}{2}\right)\right.$$
$$\left.-\frac{3}{2} + \frac{3\omega N}{4}\coth\frac{\omega N}{2}\right]$$
$$-\frac{v}{2}\int_0^N\int_0^N d\tau d\sigma\left(\frac{1}{4\pi}\right)^{3/2}A^{-3/2}\exp\left(\frac{-B^2}{4A}\right) , \tag{4.1.6}$$

where we find for $\tau > \sigma$

$$A = \frac{\sinh\frac{\omega(\tau-\sigma)}{2}\sinh\frac{\omega(N-(\tau-\sigma))}{2}}{m\omega\sinh\frac{\omega N}{2}} \qquad (4.1.7)$$

and

$$B = \frac{i.\sinh\frac{\omega(\tau-\sigma)}{2}\cosh\frac{\omega(N-(\tau+\sigma))}{2}}{\sinh\frac{\omega N}{2}}.(R_2 - R_1). \qquad (4.1.8)$$

$G_1(R_2 - R_1; N, \omega)$ is the average distribution in the first cumulant. To determine $<R^2(\tau)>$, ω must be found first. Three cases are considered:

Case I ($v = 0$ and $\omega = 0$)

This case is the free polymer chain or the chain without excluded volume effect. $\frac{\partial \ln G_1(R_2, R_1; N, \omega)}{\partial R_2} = 0$ was calculated, This approximation is equivalent to minimizing the free energy, then $R_2 = R_1$ was obtained. If one end of the polymer chain at the origin ($R_1 = 0$) is fixed and taken to the limit $\omega \to 0$ in equation (4.1.4), then

$$\left\langle R^2(\tau)\right\rangle \approx \frac{l^2(N-\tau)\tau}{N} . \qquad (4.1.9)$$

Equation (4.1.9) represents the mean square distance at any points along the chain without volume effect–free polymer chain. This result corresponds to the experiment and another methods, but is more general as can be seen for $N \to \infty$:

$$\left\langle R^2(\tau)\right\rangle \approx l^2\tau .$$

Cases II and III

In cases II and III, the variational method was used by minimizing the diagonal contribution of the exponent of $G_1(R_2 - R_1; N, \omega)$. This approximation is equivalent to minimizing the free energy:

$$\frac{\partial \ln \mathrm{Tr} G_1(R_2, R_1; N, \omega)}{\partial \omega} = 0 . \qquad (4.1.10)$$

Thus

$$\left(1-\frac{\omega N}{2}\coth\frac{\omega N}{2}\right)$$

$$+\frac{1}{2}\left(\left(\frac{\omega N}{2}\coth\frac{\omega N}{2}\right)-\left(\frac{\omega N}{2}\operatorname{cosech}\frac{\omega N}{2}\right)^2\right)=\frac{vN}{4m}\left(\frac{1}{4\pi}\right)^{3/2}\int_0^N dx A^{-5/2}$$

$$\left[\frac{\sinh\frac{\omega x}{2}\sinh\frac{\omega(N-x)}{2}}{\omega\sinh\frac{\omega N}{2}}-\frac{N\sinh^2\frac{\omega x}{2}}{2\sinh^2\frac{\omega N}{2}}\right.$$

$$\left.-\frac{x\sinh\frac{\omega(N-2x)}{2}}{2\sinh\frac{\omega N}{2}}\right], \quad (4.1.11)$$

where $x = \tau - \sigma$ and $\tau > \sigma$. Equations (4.1.6) and (4.1.11) represent a complete determination of $G_1(R_2 - R_1; N, \omega)$; however, they can not be solved exactly.

In Case II (ω is small and v is not zero):

Equation (4.1.11) was approximated as

$$1-\frac{\omega N}{4}-\frac{(\omega N)^2 e^{-\omega N}}{2}=\frac{1}{4}\left(\frac{m}{2\pi}\right)^{3/2} vN\omega^{1/2}(1+\omega N)(1-e^{-\omega N}). \quad (4.1.12)$$

By substituting equation (4.1.12) in equation (4.1.4) the following was obtaind:

$$\langle R^2\rangle = Nl^2\left[\frac{1}{4}+\frac{7vm^{3/2}N^{1/2}}{20\sqrt{2}\pi^{3/2}}-\frac{273m^3v^2N}{2000\pi^3}+\ldots\right]. \quad (4.1.13)$$

In Case III (ω is large and v is not zero):

Equation (4.1.11) can be expressed in asymptotic form as

$$\left(1-\frac{\omega N}{2}\right)+\frac{\omega N}{4}=\frac{vN}{4m}\left(\frac{1}{4\pi}\right)^{3/2}\int_0^N dx\left(\frac{1}{2m\omega}\right)^{-5/2}\left(\frac{1}{2\omega}\right)$$

$$1-\frac{\omega N}{4}=\left(\frac{vN^2}{4}\right)\left(\frac{m}{2\pi}\right)^{3/2}\omega^{3/2}$$

$$\omega=\left(\frac{2\pi}{m}\right)\left(\frac{4}{v}\right)^{2/3}N^{-4/3}\left(1-\frac{\omega N}{4}\right)^{2/3}. \quad (4.1.14)$$

Asymptotically substituting equation (4.1.14) into (4.1.4) to obtain

$$\langle R^2 \rangle \approx \left(\frac{3}{2\pi} \right) \left(\frac{\nu}{4} \right)^{2/3} N^{4/3}. \qquad (4.1.15$$

5 Discussion and Conclusions

The paper studied the polymer-excluded volume employing the Feynman pat integral method with the model proposed by Edwards. The calculation that follow is developed by us for handling the disorder system. The average mean squar displacement at any length in the polymer is obtained. Therefore the result is mor general than other methods where only the end-to-end point is calculated. In order t be able to appreciate the result of these calculations see Table 1.

Table 1.

Model Case	Perturbation	Edwards	Our method
Free chain	Nl^2	Nl^2	$\frac{l^2(N-\tau)\tau}{N}$
Weak interaction	$Nl^2\left(1+\frac{4}{3}\left(\frac{3}{2\pi l}\right)^{\frac{3}{2}}\omega L^{\frac{1}{2}}\right)$	-----	$\frac{Nl^2}{4}$
Strong interaction	------	$1.12\omega^{\frac{2}{5}}N^{\frac{6}{5}}l^{\frac{8}{5}}$	$\left(\frac{3}{2\pi}\right)\left(\frac{\nu}{4}\right)^{\frac{2}{3}}N^{\frac{4}{3}}$

Table 1: Present results are compared with the perturbation method and the method developed by Edwards. From the table for free chain all approaches lead to Nl^2. Note that since the present results give detailed information along the chain Therefore $N \to \infty$, $\frac{(N-\tau)\tau}{N} \to N$ and the present results will coincide with the free chain. For weak interaction the present results differ from the perturbation by a factor of 1/4 . This is due to our approximation by using harmonic approximation. It is well known that a harmonic approximation always leads to unphysical results for weak ω. Finally, for strong interaction the present result is $N^{4/3}$ instead of $N^{6/5}$ as

obtained by Edwards. It is noticeable that the harmonic approximation is also not very good for strong interaction. The reason is that a harmonic trial action cannot model the delta function in this excluded volume problem because the delta function has a bounded state at minus infinity. If our excluded volume has a finite range then the harmonic trial action will be able to model the long-range problem. Future research will consider more of this problem. Although the use of a harmonic trial action does not correctly produce the weak and strong coupling in the exponent, it does give the prefactor A correctly which is important for calculating the magnitude of the mean square displacement. This result can be recognized by noticing that

$$< R^2 >= AN^{\nu} .$$

Then the exponent can be obtained by plotting ν againt $\ln\left[\frac{\langle R^2\rangle}{l^2}\right]/\ln[N]$ for large N. The $<R^2>$ can be taken from equation (4.1.4) and the result is given in Fig. 1.

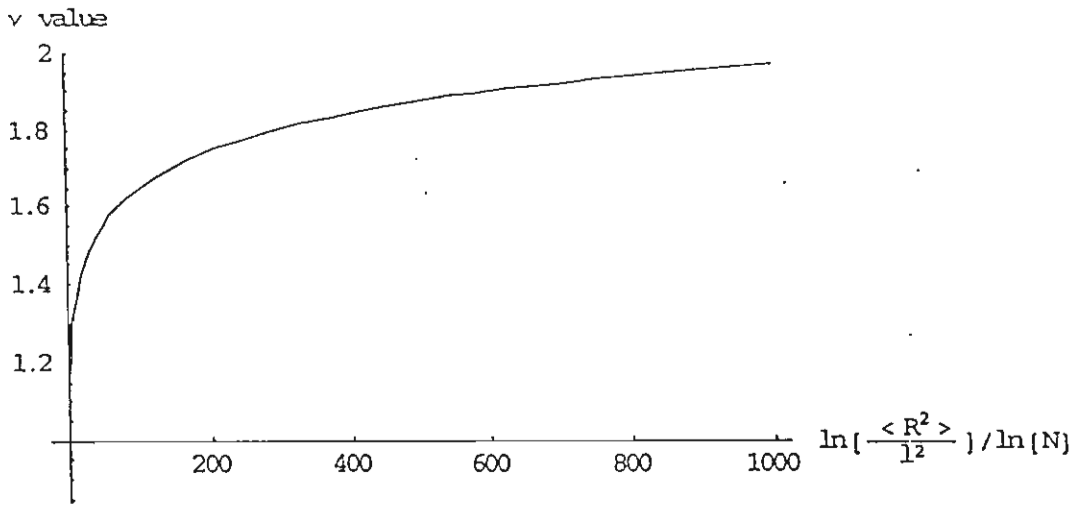

Figure 1.

The advantage of the variational method is that the mean square displacement of the polymer chain with excluded volume for any coupling strength and fluctuation along the length of the polymer can be obtained. The intermediate strength is shown graphically in Fig. 1.

Finally, this method can be generalized to two parameters as in the case of polaron.

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7 Appendix

In order to evaluate the averages of $<\mathrm{R}(\tau)>_{S_0(\omega)}$ and $<\mathrm{R}(\tau)\mathrm{R}(\sigma)>_{S_0(\omega)}$, it is nescessary to establish a characteristic functional, as

$$<\exp\left(\int_0^N d\tau \mathrm{f}(\tau)\mathrm{R}(\tau)\right)>_{S_0(\omega)}=\frac{\int_0^N D[\mathrm{R}(\tau)]\exp(-S_0(\omega)+\int_0^N d\tau \mathrm{f}(\tau).\mathrm{R}(\tau))}{\int_0^N D[\mathrm{R}(\tau)]\exp(-S_0(\omega))} \qquad \text{(A1)}$$

where $\mathrm{f}(\tau)$ is any arbitray function of time, equation (A1) suggests that if the trial action $S_0(\omega)$ is quadratic, then the action of $S_0^{'}(\omega)=S_0(\omega)-\int_0^N d\tau \mathrm{f}(\tau).\mathrm{R}(\tau)$.

Using Feynman and Hipps, the path integral of equation (A1) can be carried out exactly as

$$<\exp(\int_0^N d\tau \mathrm{f}(\tau)\mathrm{R}(\tau))>_{S_0(\omega)}=\exp\left(-\left[S_{0,cl}^{'}(\mathrm{R}_2-\mathrm{R}_1;N,\omega)-S_{0,cl}(\mathrm{R}_2-\mathrm{R}_1;N,\omega)\right]\right) \qquad \text{(A2)}$$

where $S_{0,cl}^{'}(\mathrm{R}_2-\mathrm{R}_1;N,\omega)$ and $S_{0,cl}(\mathrm{R}_2-\mathrm{R}_1;N,\omega)$ are the corresponding classical actions of $S_{0,cl}^{'}(\omega)$ and $S_{0,cl}(\omega)$. When the classical action $S_{0,cl}^{'}(\mathrm{R}_2-\mathrm{R}_1;N,\omega)$ is obtained, the classical action $S_{0,cl}(\mathrm{R}_2-\mathrm{R}_1;N,\omega)$ can be obtained form it by setting $\mathrm{f}(\tau)=0$.

To obtain the classical action $S_{0,cl}^{'}(\mathrm{R}_2-\mathrm{R}_1;N,\omega)$ a variation is required for $S_{0,cl}^{'}(\omega)$ to obtain the equation

$$\frac{d^2R_c(\tau)}{d\tau^2}-\frac{\omega^2}{N}\int_0^N d\sigma(R_c(\tau)-R_c(\sigma))=-\frac{f(\tau)}{m}. \tag{A3}$$

This equation may be rewritten in the form

$$\frac{d^2R_c(\tau)}{d\tau^2}-\omega^2R_c(\tau)=-\frac{\omega^2}{N}\int_0^N d\sigma R_c(\sigma)-\frac{f(\tau)}{m}. \tag{A4}$$

By introducing a Green Function

$$\left(\frac{d^2}{d\tau}-\omega^2\right)g(\tau,\sigma)=\delta(\tau-\sigma) \tag{A5}$$

where

$$g(\tau,\sigma)=-\left[\frac{\sinh\omega(N-\tau)\sinh\omega\sigma H(\tau-\sigma)+\sinh\omega(N-\sigma)\sinh\omega\tau H(\sigma-\tau)}{\omega\sinh\omega N}\right] \tag{A6}$$

with H denoting the Heviside step function, then the general solution of equation (A5) with the boundary condition $R(0)=R_1$ and $R(N)=R_2$ can be written as

$$R_c(\tau)=\frac{[R_2\sinh\omega\tau+R_1\sinh\omega(N-\tau)]}{\sinh\omega N}-\int_0^N\left[\frac{f(\sigma)}{m}+\frac{\omega^2}{N}\int_0^N R(\sigma)d\sigma\right]g(\tau,\sigma)d\sigma \tag{A7}$$

This equation (A7) is an integral equation which can be solved. The solution is

$$R_c(\tau)=\frac{[R_2\sinh\omega\tau+R_1\sinh\omega(N-\tau)]}{\sinh\omega N}-\int_0^N\frac{f(\sigma)}{m}g(\tau,\sigma)d\sigma$$

$$+\frac{(R_1+R_1)\sinh\frac{\omega\tau}{2}\sinh\frac{\omega(N-\tau)}{2}}{\cosh\frac{\omega N}{2}}$$

$$+\frac{4\sinh\frac{\omega\tau}{2}\sinh\frac{\omega(N-\tau)}{2}\int_0^N \mathbf{f}(\sigma)\sinh\frac{\omega\sigma}{2}\sinh\frac{\omega(N-\sigma)}{2}d\sigma}{m\omega\sinh\omega N} \tag{A8}$$

The classical action of $S_{0,cl}(\mathrm{R}_2-\mathrm{R}_1;N,\omega)$ is simply obtained by substituting R_c into the expression

$$\begin{aligned} S_0(\mathrm{R}_2-\mathrm{R}_1;\omega,N)=&\frac{m}{2}\int_0^N d\tau\,\dot{\mathrm{R}}_c^2(\tau)+\frac{m\omega^2}{4N}\int_0^N\int_0^N d\tau d\sigma(\mathrm{R}_c(\tau)-\mathrm{R}_c(\sigma))^2 \\ &-\int_0^N d\tau \mathbf{f}(\tau)\mathrm{R}_c(\tau) \\ =&\frac{m}{2}\left[\dot{\mathrm{R}}_c(N)\mathrm{R}_c(N)-\dot{\mathrm{R}}_c(0)\mathrm{R}_c(0)\right] \end{aligned} \tag{A9}$$

to give

$$\begin{aligned} S_0(\mathrm{R}_2-\mathrm{R}_1;\omega)=&\frac{m\omega}{4}\coth\frac{\omega N}{2}|\mathrm{R}_2-\mathrm{R}_1|^2 \\ &-\frac{m\omega}{2\sinh\omega N}[\frac{2\mathrm{R}_2}{m\omega}\int_0^N d\tau \mathbf{f}(\tau)\sinh\frac{\omega\tau}{2} \\ &+2\sinh\frac{\omega N}{2}\sinh\frac{\omega\tau}{2}\sinh\frac{\omega(N-\tau)}{2}) \\ &+\frac{2\mathrm{R}_1}{m\omega}\int_0^N d\tau \mathbf{f}(\tau)\sinh\frac{\omega(N-\tau)}{2} \\ &+2\sinh\frac{\omega N}{2}\sinh\frac{\omega\tau}{2}\sinh\frac{\omega(N-\tau)}{2}) \\ &+\frac{2}{m^2\omega^2}\int_0^N\int_0^\tau d\tau d\sigma \mathbf{f}(\tau)\mathbf{f}(\sigma)\sinh\omega(N-\tau)\sinh\omega\sigma \\ &+4\sinh\frac{\omega\tau}{2}\sinh\frac{\omega(N-\tau)}{2}\sinh\frac{\omega\sigma}{2}\sinh\frac{\omega(N-\sigma)}{2})] \end{aligned} \tag{A10}$$

The classical action $S_{0,cl}(\mathrm{R}_2-\mathrm{R}_1;N,\omega)$ is then obtained by setting $\mathrm{f}(\tau)=0$ in equation (A10):

$$S_0(\mathrm{R}_2-\mathrm{R}_1;\omega)=\frac{m\omega}{4}\coth\frac{\omega N}{2}\left|\mathrm{R}_2-\mathrm{R}_1\right|^2. \tag{A11}$$

Next, to evaluate the trial propagator $G_0(\mathrm{R}_1,\mathrm{R}_2;N,\omega)$, the trial action is rewritten as $S_0(\omega)$ in the form

$$S_0(\omega)=S_0(HP)-\frac{m\omega}{2N}\left(\int_0^N d\tau\mathrm{R}(\tau)\right)^2 \tag{A12}$$

where $S_0(HP)$ is the simple harmonic potential action as shown in

$$S_0(HP)=\int_0^N d\tau\frac{m}{2}\left(\dot{\mathrm{R}}^2(\tau)+\omega^2\mathrm{R}(\tau)\right). \tag{A13}$$

The second term of equation (A12) can be converted to an integral form by the identity

$$\exp\left[\frac{m\omega^2}{2N}\left(\int_0^N d\tau\mathrm{R}(\tau)\right)^2\right]=\left(\frac{N}{2\pi n\omega^2}\right)^{3/2}\int d\mathrm{f}\exp\left(\frac{-N\mathrm{f}^2}{2m\omega^2}-\int_0^N d\tau\mathrm{R}(\tau)\mathrm{f}\right). \tag{A14}$$

Form equations (A12) and (A14), it can be found that the propagator G_0 can be expressed as

$$G_0(\mathrm{R}_2,\mathrm{R}_1;N,\omega)=\left(\frac{N}{2\pi n\omega^2}\right)^{3/2}\int_{\mathrm{R}_1}^{\mathrm{R}_2}D[\mathrm{R}(\tau)]\int d\mathrm{f}\exp\left[-(S_0(HP)+\frac{N\mathrm{f}^2}{2m\omega^2}+\int_0^N d\tau\mathrm{R}(\tau)\mathrm{f})\right]. \tag{A15}$$

Changing the order of integration, (A15) becomes

$$G_0(\mathrm{R}_2,\mathrm{R}_1;N,\omega)=\left(\frac{N}{2\pi n\omega^2}\right)^{3/2}\int d\mathrm{f}\exp\left[-\frac{N\mathrm{f}^2}{2m\omega^2}\right]G_{\mathrm{f}}(\mathrm{R}_2,\mathrm{R}_1;N,\mathrm{f}) \tag{A16}$$

where

$$G_{\mathrm{f}}(\mathrm{R}_2,\mathrm{R}_1;N,\mathrm{f})=\int_{\mathrm{R}_1}^{\mathrm{R}_2}D[\mathrm{R}(\tau)]\exp\left[-(S_0(HP)+\int_0^N d\tau\mathrm{R}(\tau)\mathrm{f})\right]. \tag{A17}$$

The propagator (A17) is the force hamonic oscillator propagator with a constant external force f, which is

$$\begin{aligned}G_{\mathrm{f}}(\mathrm{R}_2,\mathrm{R}_1;N,\mathrm{f})=\left(\frac{m\omega}{2\pi\sinh\omega N}\right)^{3/2}&\exp[-(\frac{m\omega}{4}(\coth\frac{\omega N}{2}|\mathrm{R}_2-\mathrm{R}_1|^2\\&+\tanh\frac{\omega N}{2}(\mathrm{R}_2+\mathrm{R}_1)^2)+\frac{1}{\omega}\tanh\frac{\omega N}{2}(\mathrm{R}_2+\mathrm{R}_1)\mathrm{f}\\&+(\frac{1}{m\omega^3}\tanh\frac{\omega N}{2}-\frac{N\mathrm{f}^2}{2m\omega^2}))]\ .\end{aligned} \tag{A18}$$

Substituting (A18) into (A16), and performing the f-integration, equation (A19) is obtained:

$$G_0(\mathrm{R}_2,\mathrm{R}_1;N,\omega)=\left(\frac{m}{2\pi N}\right)^{3/2}\left(\frac{\omega N}{2\sinh\frac{\omega N}{2}}\right)^3\exp[-\frac{m\omega}{4}\coth\frac{\omega N}{2}|\mathrm{R}_2-\mathrm{R}_1|^2] \tag{A1}$$

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นายรังสรรค์ โกญจนาทนิกร : ฟังก์ชันการกระจายแบบคู่ในไฮโดรเจนเหลว (PAIR DISTRIBUTION FUNCTION IN LIQUID HYDROGEN) อาจารย์ที่ปรึกษา รองศาสตราจารย์ ดร. วิชิต ศรีตระกูล, 61 หน้า, ISBN 974-03-1529-1

ฟังก์ชันการกระจายแบบคู่ของโลหะเหลวไฮโดรเจน ถูกคำนวณออกมาภายใต้เงื่อนไข ความหนาแน่น ความดัน และ อุณหภูมิ ต่าง ๆ โดยวิธีการแก้สมการของ Ornstein – Zernike อาศัยการประมาณแบบ Percus – Yevick ในกรณีที่ศักย์ของอะตอมเป็นแบบทรงกลมแกร่ง ผลเฉลยที่ได้เป็นฟังก์ชันที่ขึ้นอยู่กับรัศมีทรงกลม ซึ่งสามารถคำนวณได้จากสมการสถานะเมื่อทราบ ความหนาแน่น ความดัน และอุณหภูมิ ด้วยวิธีการเดียวกันนี้เรายังคำนวณค่าปัจจัยโครงสร้าง $S(k)$ ซึ่งค่าที่ได้จะถูกนำไปใช้ในการคำนวณค่า สภาพต้านทานไฟฟ้า ตามสูตรของ Ziman จากผลการคำนวณทำให้ได้ข้อสรุปในกรณีที่ฉนวนเปลี่ยนไปเป็นโลหะด้วยการให้ความดันว่าเกิดจาก ตำแหน่งของยอดแรกของ $S(k)$ ที่เลื่อนจากจุดที่มีค่าน้อยกว่า $2k_F$ ไปสู่จุดที่มีค่ามากกว่า

ภาควิชา ฟิสิกส์ ลายมือชื่อนิสิต .....

สาขาวิชา ฟิสิกส์ ลายมือชื่ออาจารย์ที่ปรึกษา .....

ปีการศึกษา 2544 ลายมือชื่ออาจารย์ที่ปรึกษาร่วม .....

4172405623 : MAJOR PHYSICS

KEYWORD : PAIRDISTRIBUTION FUNCTION/ STRUCTURE FACTOR/ PERCUS - YEVICK

RANGSUN KONJANATNIKORN : PAIR DISTRIBUTION FUNCTION IN LIQUID HYDROGEN. THESIS ADVISOR : ASSOC. PROF. WICHIT SRITRAKOOL Ph.D., 61PP. , ISBN 974-03-1529-1.

Pair distribution function of liquid metallic hydrogen is calculated under any condition of densities, pressures, and temperatures, by using the Percus – Yevick approximation to solve the Ornstein – Zernike equation in case of hard – sphere atomic potential. The solution is dependent on the sphere radius which can be found from the equation of state when densities, pressures, and temperatures are known. By the same method, we calculate the structure factor $S(k)$ and use it to calculate the electrical resistivity following Ziman's formula. From the result, we can conclude that the insulator - metal transformation due to pressure occurs when the position of the first peak of $S(k)$ shifts from the value smaller than to the value greater than $2k_F$.

Department Physics
Field of study Physics
Academic year 2001

Student's signature .....
Advisor's signature .....
Co-advisor's signature .....

Capture radius of magnetic particles in random cylindrical matrices in high gradient magnetic separation

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An effective medium treatment (EMT) was used to model the magnetic field around randomly distributed magnetic cylindrical fine wires and applied to calculate the capture radius of paramagnetic particles in a filter operating either in the longitudinal or transverse design mode. This article reports capture radius as a function of the ratio of magnetic velocity to fluid entrance velocity with a magnetic parameter which determines the strength of the magnetic short-range force, as a parameter. Finally, comparisons of the results based on the EMT approach, with those obtained by using the single-wire model, are given along with discussion on the criteria for validity of the simple single-wire model. © *1999 American Institute of Physics.* [S0021-8979(99)00302-3]

I. INTRODUCTION

The theory of magnetic filtration has long been investigated; however, most of the theories published are based on the simplest single collector model. Among those, the formerly developed theory by Watson[1] has been referred to by many authors. This theory explains the capture of the weakly magnetic particles carried by fluid of potential flow type, defined by Reynold's number $\mathrm{Re}=\rho V_0 a/\eta \gg 1$, where ρ, V_0, η, and a are the fluid density, entrance velocity, viscosity, and collector radius, respectively. The theoretical model used consists of an isolated fine ferromagnetic cylindrical wire in the background of a uniform applied magnetic field. Later, Watson[2] calculated the capture radius of paramagnetic particles in a filter consisting of fine ferromagnetic wires using the same approach as reported in the previous publication.[1] This article includes analysis of the relation between the capture radius and the external uniform magnetic field with a magnetic parameter K_s which measures the short-range force as a parameter.

Particle capture in the random matrix at low field intensity limit has been treated by Sheerer *et al.*[3] The capture radius of a single wire with arbitrary orientation with respect to the applied magnetic field direction was evaluated and used to determine the mean capture radius in describing an overall filter efficiency. In this research, the single-wire theory is generalized and the results of Watson[2] are extended by using the effective medium treatment (EMT) to predict the magnetic field around the filter matrices consisting of parallel wires distributed randomly. The same treatment was applied to a similar system of random sphere assemblage presented by Moyer *et al.*[4,5] and Natenapit.[6] The capture radius results of this study were reported and compared with those of Watson[2] based on the single-wire model. Finally, the criteria for validity of the single-wire model used to determine magnetic field around the filter matrices are discussed.

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II. THE MAGNETIC FIELD AND FORCES

To determine the magnetic field around parallel cylindrical wires of high permeability, which are randomly distributed in a formerly uniform external magnetic field applied perpendicular to the wires' axes, the effective medium treatment originally conceived by Hashin[7] to describe the effective conductivity of spherical particulate composites was employed. In this approach, the system of magnetic cylinders and surrounding fluid medium is considered to be composed of cylindrical cells, each containing one of the cylinders. The ratio of the cylinder to cell volume (a^2/b^2) is set equal to the packing fraction of cylinders in the medium (F). Adjacent to each cylinder (permeability μ_s) is the surrounding fluid medium (permeability μ_f). In this model, only a representative cell is considered while the neighbor cells are replaced by a homogeneous medium with effective permeability μ^* to be determined. Self consistency is achieved by requiring the magnetic induction averaged over the composite cylinder (cylindrical wire plus fluid shell) to be the volume average of the magnetic induction over the effective medium[7] [see Eq. (A13)]. Taking $\mathbf{H}_0$ along x axis and the wire cross section on the xy plane, the following equations were obtained (see Appendix for details):

$$\mathbf{H}=AH_0\left[\left(1+\frac{K_c}{r_a^2}\right)\cos\theta\hat{r}-\left(1-\frac{K_c}{r_a^2}\right)\sin\theta\hat{\theta}\right],$$

$$1<r_a<\frac{b}{a} \tag{1a}$$

$$=\mathbf{H}_0, \quad \frac{b}{a}<r_a<\infty, \tag{1b}$$

where $A=1/(1-FK_c)$, $K_c=(\nu-1)/(\nu+1)$, $\nu=\mu_s/\mu_f$, and $r_a=r/a$.

Alternatively and equivalently, the effective permeability has been defined interms of the magnetic energy integral and determined by using variational theorems.[8] The consistent expression for the effective permeability μ^* has been obtained. From Eq. (1a), one can see that the magnetization

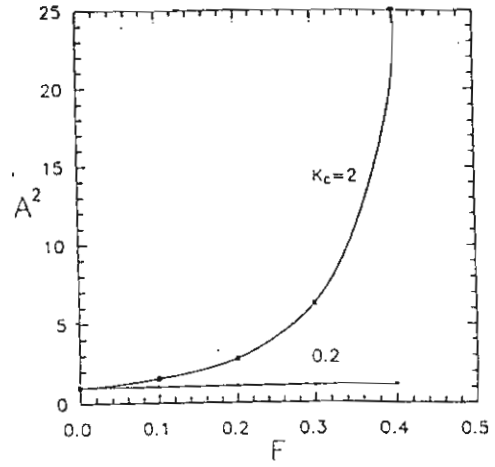

FIG. 1. A^2 as a function of packing fraction.

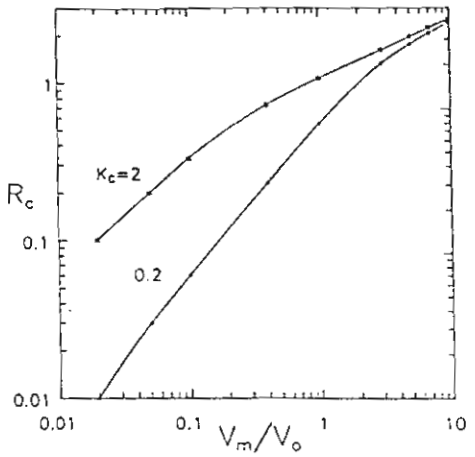

FIG. 2. Capture radius for paramagnetic particles as a function of V_m/V_0 for a longitudinal filter with packing fraction $F=0.0001$.

of the matrix increases the local field in the fluid shell, depending on the overall shape of the matrix volume and the magnetic parameter K_c. Equation (1b) is true for the EMT model used here, resulting from the boundary condition (i) in the Appendix and the obtained μ^* without further assumption on the magnetic field.

The magnetic force acting on a small particle of radius r_p and magnetic susceptibility χ_p located in the fluid of susceptibility χ_f is[9]

$$\mathbf{f}_m=\frac{2\pi}{3}r_p^3\mu_0\chi\nabla H^2, \quad \chi=\chi_p-\chi_f. \tag{2}$$

The particle is said to be paramagnetic if $\chi_p>\chi_f$ and diamagnetic if $\chi_p<\chi_f$.

Substituting H from Eq. (1) into Eq. (2), the magnetic force which depends on the particle radius, external field H_0, magnetic parameters K_c, and A^2 is obtained. Figure 1 shows the variation of A^2 as a function of the packing fraction for $K_c=0.2$ and 2. The other major force to be considered is the viscous drag force which is generally assumed to obey Stokes' law

$$\mathbf{f}_d=-6\pi\eta r_p(\mathbf{v}-\mathbf{v}_f). \tag{3}$$

Here, $\mathbf{v}_f$ is the fluid velocity, $\mathbf{v}=d\mathbf{r}/dt$ the particle velocity, and η the viscosity.

III. EQUATIONS OF MOTION

By using the magnetic field developed here and the single-wire potential flow field, the equations of motion similar to those reported by Watson[2] were obtained as follows:

$$\frac{dr_a}{dt}=\left(\frac{V_0}{a}\right)\left(1-\frac{1}{r_a^2}\right)\cos(\theta-\alpha)-\left(\frac{V_m}{a}\right)A^2\left(\frac{K_c}{r_a^5}+\frac{\cos 2\theta}{r_a^3}\right), \tag{4}$$

$$r_a\frac{d\theta}{dt}=-\left(\frac{V_0}{a}\right)\left(1+\frac{1}{r_a^2}\right)\sin(\theta-\alpha)-\left(\frac{V_m}{a}\right)A^2\frac{\sin 2\theta}{r_a^3}, \tag{5}$$

$$\frac{dz_a}{dt}=0, \tag{6}$$

where $\alpha=0$ or $\pi/2$ for a filter in longitudinal ($\mathbf{H}_0\|\mathbf{V}_0$) or transverse ($\mathbf{H}_0\perp\mathbf{V}_0$) design, respectively. Here, the magnetic velocity

$$V_m=\frac{4}{9}\frac{\chi\mu_0H_0^2r_p^2K_c}{\eta a}$$

is multiplied by the factor $A^2=1/(1-FK_c)^2$ to account for the influence of the neighboring wires on the pattern of magnetic field around the filter matrices. It is noted that the magnetic parameter K_c is equivalent to the familiar magnetic parameter $K_s=M_s/(2\mu_0H_0)$ for a single-wire model. For a normal matrix with a very low coercive force, the maximum value of $K_s=1$. $K_s>1$ can only occur for an hysteretic matrix.[10]

The equations of motion are solved numerically for particle trajectories at varying initial positions on the xy plane. The inspection of the particle trajectories yields the critical capture radius (R_c) which depends on the following parameters: V_m/V_0, F, and K_c.

IV. RESULTS AND DISCUSSION

In this research, capture radius for paramagnetic particles as a function of the ratio of magnetic velocity to fluid entrance velocity (V_m/V_0) in both longitudinal ($\mathbf{H}_0\|\mathbf{V}_0$) and transverse ($\mathbf{H}_0\perp\mathbf{V}_0$) magnetic filters with parameters $K_c=0.2$ and 2 were determined. Three cases of the magnetic filters with different values of packing fraction are considered. First, for a very dilute limit of filter packing fraction ($F=0.0001$), R_c as a function of V_m/V_0 is shown in Figs. 2 and 3. In this limit of packing fraction, $A^2\cong 1$ for all values of K_c as can be observed from Fig. 1. This indicates that the EMT results of R_c obtained are consistent with the corresponding single-wire model results reported by Watson.[2] These are confirmed for the case of magnetic filters operating in longitudinal and transverse modes as shown in Figs. 2 and 3, respectively. Furthermore, Fig. 1 also indicates that the single-wire model is a good approximation for all values of K_c up to filter packing fraction $F\sim 0.05$.

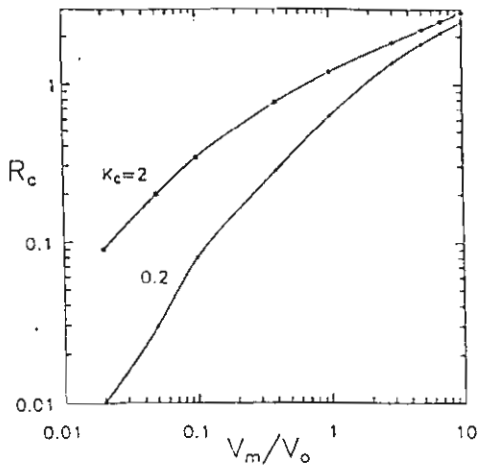

FIG. 3. Capture radius for paramagnetic particles as a function of V_m/V_0 for a transverse filter with packing fraction $F=0.0001$.

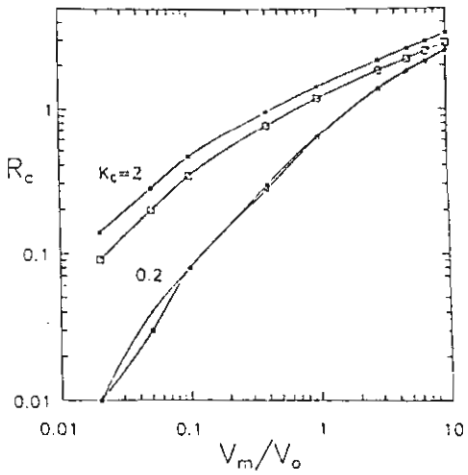

FIG. 5. Capture radius for paramagnetic particles as a function of V_m/V_0 based on EMT (*,*) and single-wire (□, □) magnetic fields for a transverse filter with packing fraction $F=0.1$.

Second, for a filter packing fraction $F=0.1$, the relation between R_c and V_m/V_0 based on the EMT magnetic field developed here, are compared with those based on the single-wire model as shown in Figs. 4 and 5 for longitudinal and transverse modes, respectively. Again two values of $K_c=0.2$ and 2 were used. For all cases, the EMT results for R_c are higher than the corresponding single-wire model results; however, the difference is insignificant for $K_c=0.2$, especially for the longitudinal mode. Thirdly, for a higher value of packing fraction ($F=0.2$), the similar dependence of R_c on V_m/V_0 are illustrated in Figs. 6 and 7 for the longitudinal and transverse modes, respectively. Here the difference between the EMT and single-wire results for $K_c=2$ is more pronounced than the former case of a lower packing fraction $F=0.1$. However, the difference is still very little for the smaller magnetic parameter $K_c=0.2$.

V. CONCLUSION

The two-dimensional description of the flow field around cylindrical matrix wires is applied to a three-dimensional problem and the geometry used is similar to that used by Kuwabara[11] to discuss the flow around cylindrical matrix wires. It should be noted that the changes in flow produced by the presence of the wire falls as r_a^{-2} and so these are considerably more important at low operating parameter V_m/V_0, than the changes in magnetic field produced by the matrix where there is a r_a^{-3} and a r_a^{-5} dependence for cylinders. In the case of spheres, the fall off is even more rapid[12] and the capture for a system of randomly packed spheres is dominated by the short-range term r_a^{-7}.

The studies also indicate that the effects of neigboring wires on the magnetic field pattern around the filter matrices may be neglected for a small packing fraction, e.g., F

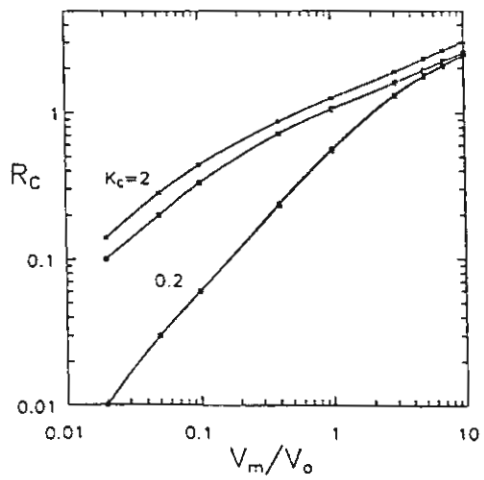

FIG. 4. Capture radius for paramagnetic particles as a function of V_m/V_0 based on EMT (*,*) and single-wire (□, □) magnetic fields for a longitudinal filter with packing fraction $F=0.1$.

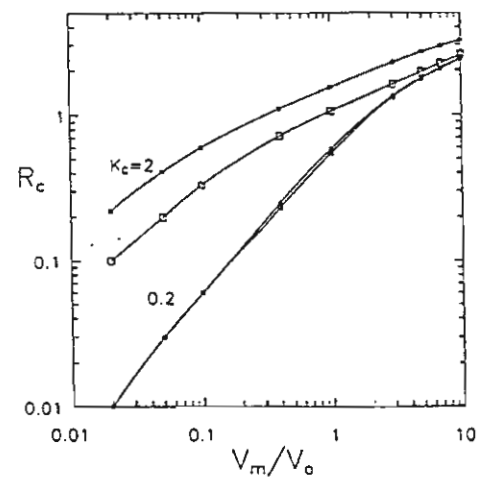

FIG. 6. Capture radius for paramagnetic particles as a function of V_m/V_0 based on EMT (*,*) and single-wire (□, □) magnetic fields for a longitudinal filter with packing fraction $F=0.2$.

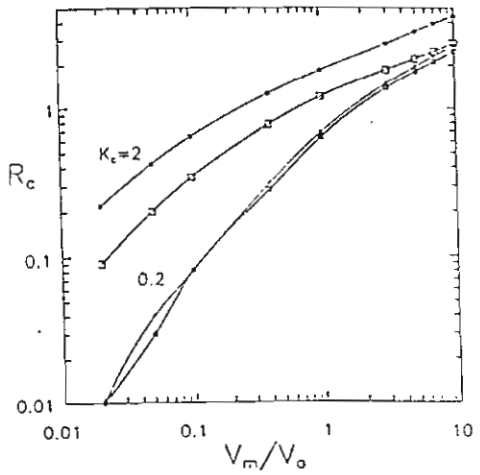

FIG. 7. Capture radius for paramagnetic particles as a function of V_m/V_0 based on EMT (•,*) and single-wire (□, □) magnetic fields for a transverse filter with packing fraction $F=0.2$.

$\cong 0.05$, for all possible values of the magnetic parameter K_c which determines the strength of the magnetic short-range force [r_a^{-5} term in Eq. (4)]. Here K_c depends on the ratio of the wire permeability to fluid permeability as $K_c=(\mu_s/\mu_f-1)/(\mu_s/\mu_f+1)$. However, for a higher packing fraction, the single-wire approximation is still good only for the lower values of K_c (say <0.2).

ACKNOWLEDGMENTS

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APPENDIX

To determine the magnetic field in the cell, the boundary value problem of coaxial magnetic cylinders subject to the boundary condition of uniform magnetic field at far away from the cylindrical cell is solved. Taking z axis of cylindrical coordinate along the cylinder axis and let φ be the magnetic potential satisfying Laplace's equation for each region

$$\nabla^2\varphi_0=0, \quad b<r<\infty, \tag{A1}$$

$$\nabla^2\varphi_1=0, \quad a<r<b, \tag{A2}$$

$$\nabla^2\varphi_2=0, \quad 0<r<a \tag{A3}$$

with the boundary conditions

(i) $\varphi_0(r,\theta)=-H_0 r\cos\theta$ at $r\to\infty$,

(ii) $\dfrac{\partial\varphi_0(b,\theta)}{\partial\theta}=\dfrac{\partial\varphi_1(b,\theta)}{\partial\theta}$,

(iii) $\dfrac{\partial\varphi_1(a,\theta)}{\partial\theta}=\dfrac{\partial\varphi_2(a,\theta)}{\partial\theta}$,

(iv) $\mu^*\left.\dfrac{\partial\varphi_0(r,\theta)}{\partial r}\right|_{r=b}=\mu_f\left.\dfrac{\partial\varphi_1(r,\theta)}{\partial r}\right|_{r=b}$,

and

(v) $\mu_f\left.\dfrac{\partial\varphi_1(r,\theta)}{\partial r}\right|_{r=a}=\mu_s\left.\dfrac{\partial\varphi_2(r,\theta)}{\partial r}\right|_{r=a}$.

The general solutions of Laplace's Eqs. (A1)–(A3) are

$$\varphi_0(r,\theta)=-H_0 r\cos\theta+\sum_{n=1}^{\infty}A_n r^{-n}\cos n\theta, \tag{A4}$$

$$\varphi_1(r,\theta)=\sum_{n=1}^{\infty}[B_n r^n+C_n r^{-n}]\cos n\theta, \tag{A5}$$

and

$$\varphi_2(r,\theta)=\sum_{n=1}^{\infty}D_n r^n\cos n\theta, \tag{A6}$$

where the boundary condition (i) was imposed.

Applying the boundary conditions (ii)–(v), the constant coefficients were obtained as follows:

$$A_n=B_n=C_n=D_n=0, \quad \text{for } n\neq 1, \tag{A7}$$

$$A_1=\frac{H_0a^2}{lF}[F(\nu^*+1)(\nu-1)-(\nu^*-1)(\nu+1)], \tag{A8}$$

$$B_1=-\frac{2H_0\nu^*}{l}(\nu+1), \tag{A9}$$

$$C_1=\frac{2H_0a^2\nu^*}{l}(\nu-1), \tag{A10}$$

and

$$D_1=-\frac{4H_0\nu^*}{l}, \tag{A11}$$

where $\nu^*=\mu^*/\mu_f$, $\nu=\mu_s/\mu_f$, and $l=[(\nu^*+1)(\nu+1)-F(\nu-1)(\nu^*-1)]$.

The magnetic field related to φ by

$$\mathbf{H}=-\nabla\varphi \tag{A12}$$

is now obtained everywhere by inserting Eqs. (A4)–(A11) into the above equation. However, the results are given interms of the unknown effective permeability μ^*. μ^* is determined self consistency by requiring the magnetic induction averaged over the composite cell (cylinder plus cell medium) to be the volume average of the magnetic induction over the effective medium. That is,

$$F\mu_s\langle H_2\rangle_i+(1-F)\mu_f\langle H_1\rangle_i=\mu^*\langle H_{\text{eff}}\rangle_i, \quad (H_{\text{eff}}=-\nabla\varphi_0), \tag{A13}$$

where i referred to x, y, or z. Substituting the magnetic field into Eq. (A13) and taking the x component, we obtain the relative effective permeability

$$\nu^*=\frac{\nu(1+F)+(1-F)}{\nu(1-F)+(1+F)}, \quad \left(\nu^*=\frac{\mu^*}{\mu_f},\nu=\frac{\mu_s}{\mu_f}\right). \tag{A14}$$

Then, the magnetic fields in the cell and the effective medium are obtained as

$$\mathbf{H}=AH_0\left[\left(1+\frac{K_c}{r_a^2}\right)\cos\theta\hat{r}-\left(1-\frac{K_c}{r_a^2}\right)\sin\theta\hat{\theta}\right],$$

$$1<r_a<\frac{b}{a} \tag{A15a}$$

$$=H_0, \quad b/a<r_a<\infty, \tag{A15b}$$

where $A=1/(1-FK_c)$, $K_c=(\nu-1)/(\nu+1)$, and $r_a=r/a$.

We note that in the limit of $F(=a^2/b^2)\to 0$, $\nu^*=1$ (or $\mu^*=\mu_f$), and Eq. (A15a) is reduced to the single cylinder solution as expected. For $\mu_s=\mu_f$ (i.e. $K_c=0$, $A=1$), the homogeneous magnetic field $\mathbf{H}=H_0$ is obtained.

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Electronic transport properties of Sierpinski lattices

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We have studied the electronic transport properties of open Sierpinski gasket systems connected to two electron reservoirs in the presence of a magnetic field. In the framework of a tight-binding model, the systems are composed of one-dimensional ordered chains. A generalized eigenfunction method, which allows one to deal with finite systems consisting of a large number of lattice sites (nodes), is used to calculate the transmission and reflection coefficients of the studied systems. The numerical results show that there are two kinds of symmetries of the transmission coefficient T to magnetic flux Φ, and there are antiresonant state regions ($T=0$) and resonant states ($T=1$). It is different from the open ring systems now the electronic energies of resonant states do not coincide with the eigenenergies of the isolated Sierpinski gasket systems. It is also found that the transmission behavior of the single exit systems is much more complicated than that of two exit systems. [S0163-1829(99)03640-1]

I. INTRODUCTION

In the past decade, rapid progress has been made in the area of mesoscopic physics. Quantum transport in mesoscopic systems has been extensively studied both experimentally and theoretically.[1–19] For mesoscopic systems at very low temperatures, the scattering due to phonons, which is a dephasing scattering, is significantly suppressed and the phase-coherence length of electrons becomes large compared to the system dimension. The scattering in the systems can then be modeled as phase-coherent elastic scatterings. Furthermore, if we consider the electron as a free particle, an idealized sample becomes an electron waveguide, which assumes that the electron transport through the system is perfectly ballistic. In recent years, there have been many works devoted to the study of the electronic properties of mesoscopic systems within the framework of the waveguide theory[9–14] and the tight-binding model.[7,8,15–19] Along these lines, the theoretical work to date has focused largely on the problems related to an isolated ring, or to open ring systems connected via leads to electronic reservoirs together with a magnetic flux Φ through the rings. For an isolated ring, the persistent current has been the focus of attention.[3–6] The idea is based on the possibility that the electron wave function may extend coherently over the whole circumference of the ring, and elastic scatterings, finite temperature, and weak inelastic scatterings do not destroy the coherence. As for the open ring systems, the important problem is to study the relationship among the transmission coefficient T, incident electron energy E, and magnetic flux Φ through the rings. The electron reservoirs in the open ring systems act as the source of energy dissipation or irreversibility, and all scattering processes in the leads and rings are assumed to be elastic. Based on the waveguide theory, Xia[10] has studied the Aharonov-Bohm effect in an open ring by calculating the transmission and reflection amplitudes as functions of the magnetic flux, the arm length, and the wave vector. Singha Deo and Jayannavar[12,13] have studied the quantum transport properties of serial stub or ring structures and the band formation in these geometries. Takai and Ohta[14] have published a series of articles investigating similar problems in the presence of both an electrostatic potential and magnetic flux.

On the other hand, it is well known that the tight-binding model is more flexible in theoretical treatments than the waveguide theory as disorder can be introduced readily and the band-structure effects are included.[20,21] Along these lines, Entin-Wohlman *et al.*[7] and Kowal *et al.*[8] have studied the electronic transport properties of an open single ring. Aldea *et al.*[11] studied the same problems using the Green's-function method. Wu and Mahler[9] have developed the quantum network theory of transport, by which the transmission probability for an open A-B type ring with an arbitrary form factor has been studied in detail. Liu and co-workers have investigated the persistent current of an isolated disordered ring,[15] the effects of spin interaction on the persistent current,[16] as well as the electronic transport properties of variant ring systems threaded by magnetic flux.[17–19]

Fractals and their properties have been studied by physicists for many years. Lakhtakia *et al.* have studied the construction and the analytic properties of the fractal clusters, and they also investigated the diffusion motion of the Pascal-Sierpinski gaskets by using combinational algebra.[20] For electronic transmission, the fractal lattices are much more complicated in structure compared with the ring systems. One of the main points of interest has been the fact that these self-similar objects are found to serve as a nontrivial model

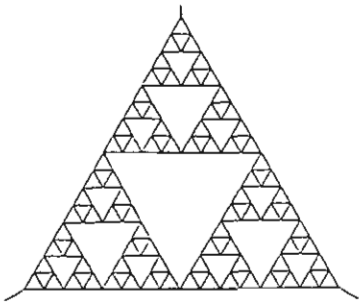

FIG. 1. The fourth-generation Sierpinski gasket lattice, the electronic properties of which are studied in the text.

for the backbone of transport problems. Fractals, in particular deterministic fractals such as the Sierpinski gasket (SG) fractal, possess some special properties, one of which is scale invariance, and do not have any translational order. They in fact bridge the gap between periodic and disordered systems.[22] Therefore, a detailed study on the electronic properties of fractals would lead to new physical results and increase our understanding of nonperiodic systems. Even though there is a large volume in the literature concerned with fractal systems, the study of their electronic properties is not that exhaustive. Along these lines, the energy spectrum and localization of electronic states in an isolated Sierpinski gasket lattice (SGL) have been the subject of many papers.[23–27] Domany *et al.*[23] studied the energy spectrum of the isolated SGL by the use of the recursive technique. Rammal and Toulouse[24] investigated the same problem in the presence of a magnetic field. However, in recent years the belief has been that in a highly correlated self-similar fractal system, such as SGL, localized eigenstates can exist. This should be a kind of structure-induced localization, which is different from Anderson localization due to incoherent scattering.[21] Therefore, the electronic transport properties of this kind of fractal structure would be an interesting problem. Chakrabarti[26] has found that in the absence of magnetic field for the isolated SGL, there are extended electron states. Wang[27] has studied the electronic localization of Sierpinski lattices, and claimed that there exist an infinite number of extended states. He has also studied the magnetic-field effects on the electronic states of the isolated SGL. But to the best of our knowledge, up to now the study on the electronic transport properties of an open SGL has not been reported yet. The reason would be that to deal with an electronic transmission problem of an open SGL, one would have to solve a united equation set, in which the number of equations roughly equals the number of the sites included in the SGL. Therefore, even for a finite SGL, this is a difficult work. Fortunately, we have found an effective approach to solve this problem, in which the transmission and reflection amplitudes are treated together with the electronic wave functions in the sites of the SGL, so that we can deduce a simpler formula to calculate the transmission and reflection coefficients. We have named this approach the generalized eigenfunction method (GEM). By the use of this GEM we have investigated the electronic transport properties of open SGL up to its fourth-generation system containing 123 sites (nodes), which is shown in Fig. 1. By the way, this GEM is formally similar to the fast multipole method (FMM), which is commonly used in electromagnetic scattering problems, but we should point out that they are essentially different from each other.[28] The main purpose of this paper is to investigate the behavior of the transmission coefficient T as the incident electron energy E and the magnetic flux Φ, which penetrates the elementary triangles of the SGL, are varied. Detailed results are given in three-dimensional plots of T against E and Φ, and of which in the two-dimensional cross sections T versus E. It is found that there are two kinds of symmetries of transmission coefficient T to flux Φ. The transmission behavior of single-exit SGL systems is much more complicated than that of two-exit systems. We also found that as the SGL generation increases, the antiresonant regions corresponding to $T=0$ in the E-Φ space progressively increase in both the region number and the region area. This means that in these regions the magnetic flux completely blocks out the electronic transport. This is an interesting quantum phenomenon. On the other hand, we have also calculated the eigenenergy spectrum of the corresponding isolated SGL, and found that in the open SGL case the electron energies of resonant transmission states do not coincide with the eigenenergies of the isolated SGL, which is different from the open ring systems.[18]

This paper is organized as follows. In Sec. II, we introduce the generalized eigenfunction method (GEM) to calculate the transmission and reflection coefficients of an open SGL. The numerical results and discussion of the electronic transport properties are presented in Sec. III. A brief summary is given in Sec. IV.

II. GENERALIZED EIGENFUNCTION METHOD AND ITS APPLICATION IN OPEN SGL SYSTEMS

For the studied open Sierpinski gasket lattices (SGL) which are coupled to two reservoirs via ideal leads, we assume that the leads connected to neighboring sites are composed of one-dimensional ordered chains with on-site energy ε_n and transfer integral t between nearest-neighboring sites. Denoting the incident electron energy by E and the projection of the Wannier wave function on the nth site by ψ_n, in the presence of a magnetic flux Φ the tight-binding equation can be written as[19]

$$(\varepsilon_n - E)\psi_n = \sum_{n'} t_{n,n'}\psi_{n+n'}, \tag{1}$$

where the transfer integral $t_{n,n'}$ equals $te^{\pm i2\pi\Phi/(\Phi_0 S)}$, the $S=3$ is the circumference length of the elementary triangle of the SGL, the magnetic phase $\phi=2\pi\Phi/(\Phi_0 S)$, the $\Phi_0=hc/e$ is the elementary flux quantum, and the sum runs over the nearest neighbors of site n. The wave function ψ_n can be written as the linear combination[18]

$$\psi_n = Ae^{ikn} + Be^{-ikn}, \tag{2}$$

where k is the wave vector, n is the site number, and we take the lattice distance to be unity. In the tight-binding model, the wave vector k is related with the incident electronic en-

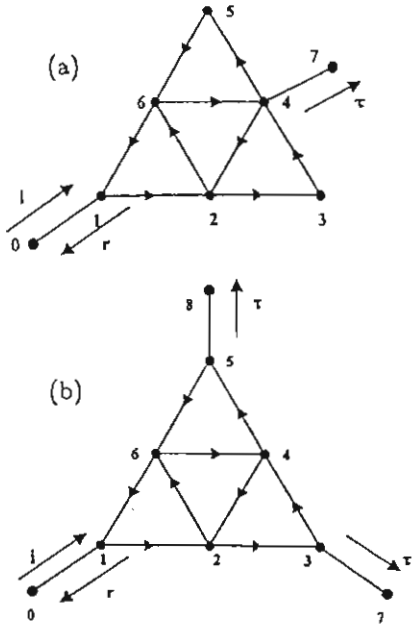

FIG. 2. First-generation Sierpinski lattice coupled to two reservoirs via ideal leads. The magnetic phase is equal to ϕ in the direction of the arrow and $-\phi$ otherwise. (a) One-exit case. (b) Two-exit case; both exits are coupled to the same reservoirs via ideal leads.

ergy E by formula $E=2t\cos k$. We first consider the first-generation SGL with a single exit shown in Fig. 2(a). By the use of Eq. (1) we obtain the tight-binding equations on the sites of the SGL as follows:

$$E\psi_1=te^{-i\phi}\psi_2+te^{-i\phi}\psi_6+t\psi_0,$$

$$E\psi_2=te^{i\phi}\psi_1+te^{-i\phi}\psi_3+te^{i\phi}\psi_4+te^{-i\phi}\psi_6,$$

$$E\psi_3=te^{i\phi}\psi_2+te^{-i\phi}\psi_4,$$

$$E\psi_4=te^{-i\phi}\psi_2+te^{i\phi}\psi_3+te^{-i\phi}\psi_5+te^{i\phi}\psi_6+t\psi_7, \tag{3}$$

$$E\psi_5=te^{i\phi}\psi_4+te^{-i\phi}\psi_6,$$

$$E\psi_6=te^{-i\phi}\psi_1+te^{i\phi}\psi_2+te^{-i\phi}\psi_4+te^{i\phi}\psi_5.$$

On the other hand, for the special sites located in the entry and exit we can write their wave function as[19]

$$\psi_0=1+r \quad (n=0),$$

$$\psi_1=e^{ik}+re^{-ik} \quad (n=1),$$

$$\psi_4=\tau \quad (n=0), \tag{4}$$

$$\psi_7=\tau e^{ik} \quad (n=1),$$

where r and τ are the reflection and transmission amplitudes of reflecting and outgoing wave functions, respectively. To calculate both of them, we have to solve the above united equation set (3) and (4); evidently this is difficult. If we consider higher-generation SGL, then obtaining an analytic solution seems impossible. To numerically solve this problem, we introduce the following generalized eigenfunction method (GEM). The trick of the GEM is that we treat the amplitudes r and τ the same as the wave functions ψ_i. In this way the united equation set (3) and (4) can be rewritten as the following $(N+2)$-order matrix equation. N is the number of sites in the SGL:

$$\begin{bmatrix} E & e^{-i\phi} & 0 & 0 & 0 & e^{i\phi} & 1 & 0 \\ e^{i\phi} & E & e^{-i\phi} & e^{i\phi} & 0 & e^{-i\phi} & 0 & 0 \\ 0 & e^{i\phi} & E & e^{-i\phi} & 0 & 0 & 0 & 0 \\ 0 & e^{-i\phi} & e^{i\phi} & E & e^{-i\phi} & e^{i\phi} & 0 & e^{ik} \\ 0 & 0 & 0 & e^{i\phi} & E & e^{-i\phi} & 0 & 0 \\ e^{-i\phi} & e^{i\phi} & 0 & e^{-i\phi} & e^{i\phi} & E & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & -e^{-ik} & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & -1 \end{bmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \\ \psi_5 \\ \psi_6 \\ r \\ \tau \end{pmatrix} = \begin{pmatrix} -1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ e^{ik} \\ 0 \end{pmatrix}. \tag{5}$$

For the sake of simplicity, in the above equation we have chosen $\varepsilon_n=0$ and $t=1$.

If we denote the above matrix equation (5) as

$$M\Psi=C,$$

then the reflection and transmission amplitudes are simply

$$r=(M^{-1}C)_{N+1}, \quad \tau=(M^{-1}C)_{N+2}, \tag{6}$$

and the transmission coefficient $T=|\tau|^2$.

Here we would like to emphasize two points. First, the numerical solution of the above formula (6) is very easy to obtain even with a personal computer. Second, the above generalized eigenfunction method is a very powerful approach to deal with the electronic transport problems in lattice (network) systems, no matter how many entries and exits exist in the studied systems. Even for the quasiperiodic and disordered ones, and for three-dimensional systems, this GEM can also be very efficiently used. For example, the matrix equation of the first-generation SGL with *two exits* shown in Fig. 2(b) can be easily written as follows:

$$\begin{bmatrix} E & e^{-i\phi} & 0 & 0 & 0 & e^{i\phi} & 1 & 0 & 0 \\ e^{i\phi} & E & e^{-i\phi} & e^{i\phi} & 0 & e^{-i\phi} & 0 & 0 & 0 \\ 0 & e^{i\phi} & E & e^{-i\phi} & 0 & 0 & 0 & e^{ik} & 0 \\ 0 & e^{-i\phi} & e^{i\phi} & E & e^{-i\phi} & e^{i\phi} & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{i\phi} & E & -i\phi & 0 & 0 & e^{ik} \\ e^{-i\phi} & e^{i\phi} & 0 & e^{-i\phi} & e^{i\phi} & E & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & -e^{-ik} & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -1 \end{bmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \\ \psi_5 \\ \psi_6 \\ r \\ \tau_1 \\ \tau_2 \end{pmatrix} = \begin{pmatrix} -1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ e^{ik} \\ 0 \\ 0 \end{pmatrix}, \tag{7}$$

which is now an $(N+3)$-order matrix equation. In deducing the above matrix equation (7) we have used the following relations held in sites 3 and 5 of Fig. 2(b):

$$E\psi_3 = te^{i\phi}\psi_2 + te^{-i\phi}\psi_7 + t\tau_1 e^{ik},$$

$$E\psi_5 = te^{i\phi}\psi_4 + te^{-i\phi}\psi_6 + t\tau_2 e^{ik}.$$

The corresponding reflection and transmission amplitudes of reflecting and outgoing wave functions are, respectively,

$$r = (M^{-1}C)_{N+1}, \quad \tau_1 = (M^{-1}C)_{N+2}, \quad \tau_2 = (M^{-1}C)_{N+3}. \tag{8}$$

From the above example we can see that in the same way we can easily extend the GEM to multientries (and exits) cases. To clarify the name GEM, we should compare the generalized eigenfunction equation (5) with the energy eigenvalue matrix equation of an *isolated* SGL written in the following. If we assume the site energy $\epsilon_n = 0$ for the whole system, then the tight-binding equations in the sites and their corresponding eigenvalue matrix equation are, respectively,

$$E\psi_1 = te^{-i\phi}\psi_2 + te^{-i\phi}\psi_6,$$

$$E\psi_2 = te^{i\phi}\psi_1 + te^{-i\phi}\psi_3 + te^{i\phi}\psi_4 + te^{-i\phi}\psi_6,$$

$$E\psi_3 = te^{i\phi}\psi_2 + te^{-i\phi}\psi_4,$$

$$E\psi_4 = te^{-i\phi}\psi_2 + te^{i\phi}\psi_3 + te^{-i\phi}\psi_5 + te^{i\phi}\psi_6, \tag{9}$$

$$E\psi_5 = te^{i\phi}\psi_4 + te^{-i\phi}\psi_6,$$

$$E\psi_6 = te^{-i\phi}\psi_1 + te^{i\phi}\psi_2 + te^{-i\phi}\psi_4 + te^{i\phi}\psi_5,$$

and

$$\begin{bmatrix} E & e^{-i\phi} & 0 & 0 & 0 & e^{i\phi} \\ e^{i\phi} & E & e^{-i\phi} & e^{i\phi} & 0 & -i\phi \\ 0 & e^{i\phi} & E & e^{-i\phi} & 0 & 0 \\ 0 & e^{-i\phi} & e^{i\phi} & E & e^{-i\phi} & e^{i\phi} \\ 0 & 0 & 0 & e^{i\phi} & E & e^{-i\phi} \\ e^{-i\phi} & e^{i\phi} & 0 & e^{-i\phi} & e^{i\phi} & E \end{bmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \\ \psi_5 \\ \psi_6 \end{pmatrix} = 0, \tag{10}$$

where we can see that the above N-order square matrix is the submatrix of matrix $\mathbf{M}$ of the matrix equation (5), and the above eigenwave function vector is the subvector of the corresponding vector of matrix equation (5). That is why we call the method the generalized eigenfunction method.

III. NUMERICAL RESULTS AND DISCUSSION

The formalism mentioned in Sec. II can be easily implemented numerically and the results for both the single- and two-exit cases are obtained up to fourth-generation open SGL with site (node) number $N = 123$. The numerical calculation is easy and quick even with a personal computer. Because the main characters of the transport properties have been revealed in the investigation of the first four generation SGL, it is not necessary to consider the higher-generation systems. In our calculations, the on-site energies are chosen to be $\epsilon_n = 0$ and the transfer integrals $t = -1.0$. To examine the accuracy of our numerical calculations, we check at every intermediate stage of the calculation that the criterion $|\tau|^2 + |r|^2 = 1$ for the transmission and reflection coefficients is satisfied to a tolerance of 10^{-14}. This accuracy enables us to examine with confidence the electronic transport properties of the open SGL.

We consider two basic cases of the open SGL with one and two exits, of which the first-generation systems are

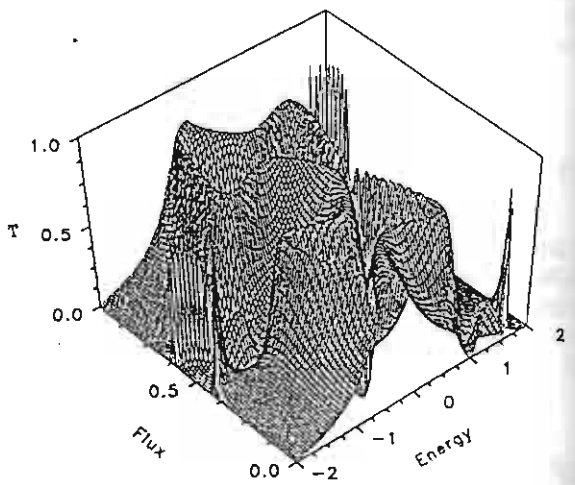

FIG. 3. Transmission coefficient T as a function of magnetic flux Φ and incident electron energy E for the first-generation Sierpinski lattice with a single exit.

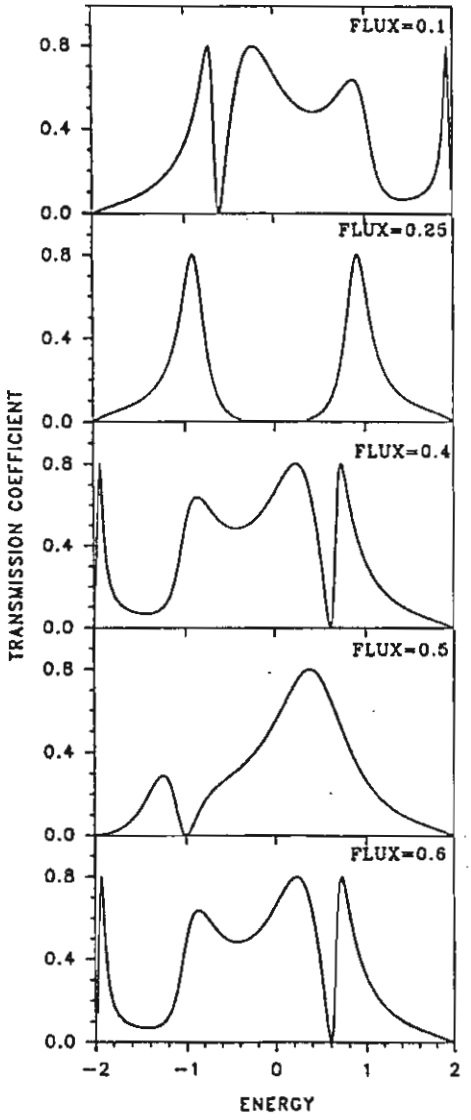

FIG. 4. Transmission coefficient T vs electron energy E as cross sections of Fig. 3. The corresponding flux is marked in the pictures. The two pictures are the same for $\Phi/\Phi_0=0.4$ and 0.6, but for $\Phi/\Phi_0=0.1$ and 0.4 they are "antisymmetric" to energy E (see text).

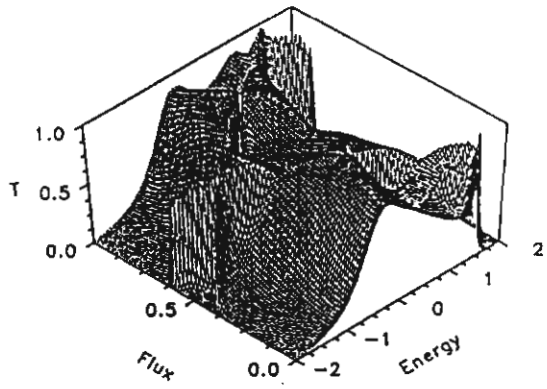

FIG. 5. Transmission coefficient T as a function of magnetic flux Φ and incident electron energy E for first-generation Sierpinski lattice with two exits.

shown in Fig. 2. By the use of the GEM, we have totally calculated the first four generation SGL. The numerical results are shown in Figs. 3–11, in which the typical three-dimensional plots of the transmission coefficient T against the electron energy E and magnetic flux Φ are shown in Figs. 3 and 5 for the first-generation SGL, in Figs. 7 and 8 for the second-generation SGL, in Fig. 10 for the third-generation SGL, and in Fig. 11 for the fourth-generation SGL. For the sake of clear visualization and because of the symmetry of the transmission spectrum, we plotted only a half and a quarter of the whole periodic picture in Figs. 10 and 11, respectively. To display the detail, we have also plotted some pictures of the transmission coefficient T versus energy E, i.e., the cross sections of three-dimensional plots, for the first-generation SGL in Fig. 4 (single exit) and Fig. 6 (two exits), and for the second-generation SGL with two exits in Fig. 9.

From the obtained numerical results, we can see some interesting transport properties, which exist in all studied SGL cases. First, following the enlargement of the SGL, the transmission coefficient T fluctuates more and more, i.e., there exist more and more peaks, valleys, and more and bigger zero-transmission ($T=0$) regions. This complexity of the transmission behaviors can be understood as the result of the quantum coherence effect among electrons traveling through the SGL. This is due to the fact that the presence of a magnetic flux destroys the time-reversal symmetry and the paths going clockwise and anticlockwise over the systems have different phases. Therefore, when the site number of the systems increases, the variant possibility of quantum coherence also increases, and the transmission coefficient as a function of the electron energy E and magnetic flux Φ becomes increasingly complicated. For the same reason, from the figures we can also see that the antiresonant state region, i.e., the region with $T=0$, enlarges following the increase of the site number. In Figs. 3 and 5 of the first-generation SGL there is no such region, but one does appear in Figs. 7 and 8 of the second-generation SGL and enlarges in the next generations. In the fourth generation SGL several such regions have appeared and their areas have quickly enlarged (see Fig. 11). This global behavior is clearly displayed in the three-dimensional T-E-Φ plots. To show the sophisticated relationship between the incident electron energy and its transmission coefficient, we have plotted the E versus T curves with $\Phi/\Phi_0=0.1$, 0.25, 0.4, 0.5, and 0.6, respectively, for the first- and second-generation SGL, and shown them in Figs. 4, 6, and 9, which compliment very well their corresponding 3D plots.

Second, we have noticed the symmetry of transmission behaviors. Because we need to use the eigenvalue matrix equation (10) to discuss the parameter symmetry of the transport property, we investigate in advance the relationship between the resonant electronic states of the *open* SGL and the energy eigenvalues of the *isolated* SGL. An incident electronic state with peak-value transmission coefficient T is called a resonant state. In the open ring systems the electronic energies of resonant states are close to the eigenenergies of the corresponding isolated ring systems.[18] An inter-

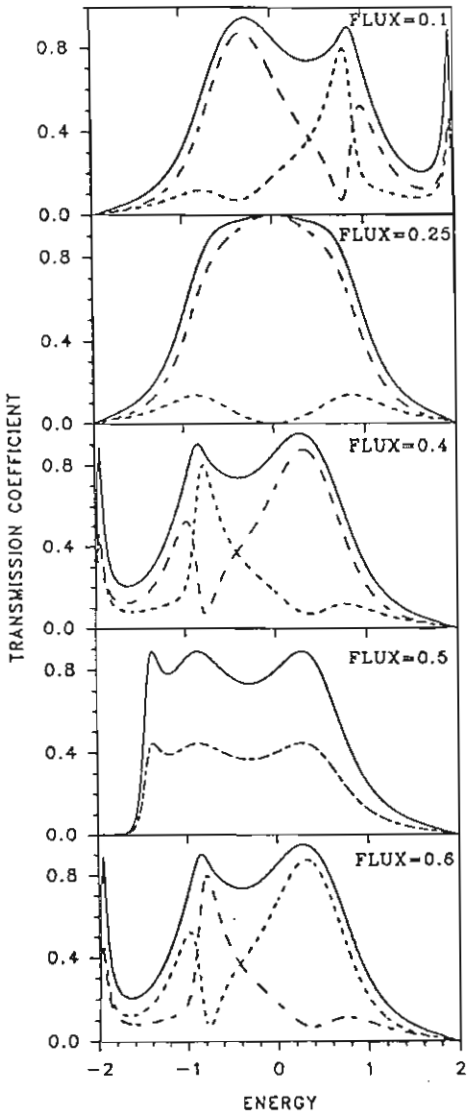

FIG. 6. Transmission coefficient T vs electron energy E as cross sections of Fig. 5. The corresponding flux is marked in the pictures. Long- and short-dashed lines are the transmission coefficients of exits 7 and 8, respectively. Solid lines are the sum of them. The plots show the same symmetry as the single-exit case (see text).

esting question is whether or not there exists the same kind of relationship in the SGL systems. Figure 12 shows the energy eigenvalue spectra of the isolated Sierpinski lattice for the first, second, and fourth generations, which are obtained by calculating Eq. (10). Comparing Fig. 12 with Figs. 3, 5, 7, 8, and 11, which show the T-Φ-E behaviors, we can see that in both the single- and two-exit cases, there is no definite correspondence between the electron energy of the resonant states of the open SGL and the eigenenergy of the isolated SGL. This means that the transport properties of the fractal systems are more complicated than those of the slab systems[13–14] and ring systems.[18] A plausible explanation for this phenomenon should be that the structure of the fractal systems is much more complicated than that of the ring systems, which leads to many more possibilities of variant reflection and transmission, so that quantum coherence effects have a much greater chance to influence the transport properties and finally destroy the correspondence of the two kinds of energies that exist in the open ring systems.

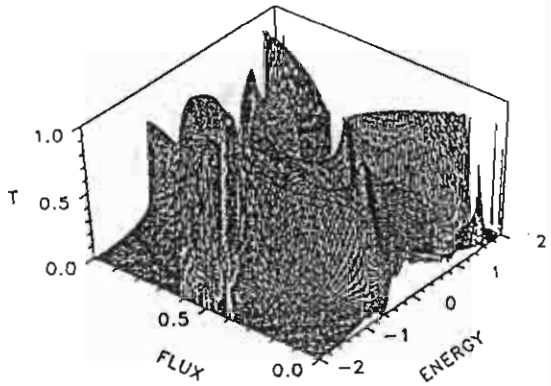

FIG. 7. Transmission coefficient T as a function of magnetic flux Φ and incident electron energy E for second-generation Sierpinski lattice with single exit.

On the other hand, from the energy spectra shown in Fig. 12 we have noticed that there are two kinds of symmetries. First, the energy spectrum is symmetric to $\Phi/\Phi_0=0.5$, i.e., for fluxes Φ/Φ_0 and $1-\Phi/\Phi_0$ two energy bands are exactly the same. Second, to the $\Phi/\Phi_0=0.25$ (or 0.75) the energy spectrum is "antisymmetric," i.e., there is a correspondence between $E(\Phi/\Phi_0)$ and $-E(0.5-\Phi/\Phi_0)$ for $\Phi/\Phi_0 \leq 0.25$. This symmetrization of the energy spectrum could be understood from the eigenequation (10) of the first-generation SGL. We have obtained the polynomial expression satisfied by eigenenergies E:

$$-2-\cos 6\phi+6E\cos 3\phi-56E^3\cos 3\phi-480E^4+512E^6 = 0, \tag{11}$$

from which we can see that the symmetry of the eigenenergy spectrum depends on the symmetry of $\cos 3\phi$, where

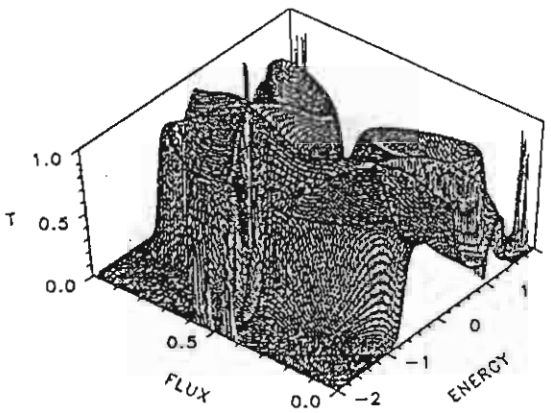

FIG. 8. Transmission coefficient T as a function of magnetic flux Φ and incident electron energy E for second-generation Sierpinski lattice with two exits.

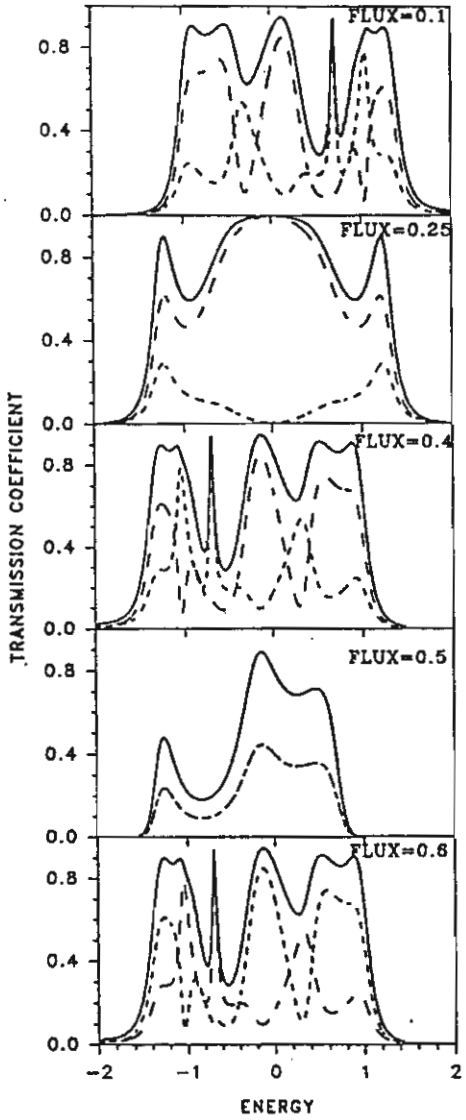

FIG. 9. Transmission coefficient T vs electron energy E as cross sections of Fig. 8. The corresponding flux is marked in the pictures. Long- and short-dashed lines are the transmission coefficients of exits 7 and 8, respectively. Solid lines are the sum of them. The plots show the same symmetry as the first-generation case (see text).

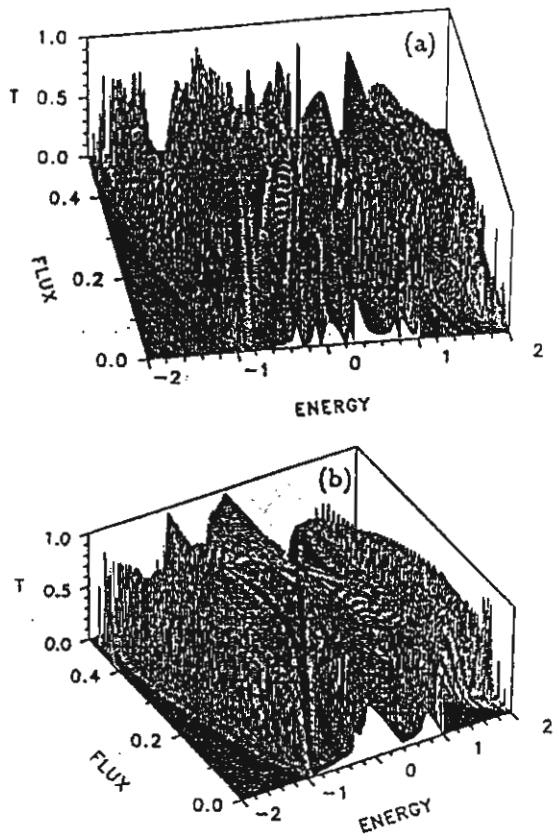

FIG. 10. Transmission coefficient T as a function of magnetic flux Φ and incident electron energy E for third-generation Sierpinski lattice. For the sake of clear visualization only a half-period in flux Φ is shown. (a) Single-exit case. (b) Two-exit case.

$\phi=2\pi\Phi/3\Phi_0$ so that $\cos 3\phi=\cos 2\pi\Phi/\Phi_0$. This is why there are $\Phi/\Phi_0=0.5$ and $\Phi/\Phi_0=0.25$ (0.75) kinds of symmetries, because they are merely the symmetries of $\cos 3\phi$. Here we can also see that the energy spectrum is periodic in flux with period $\Phi/\Phi_0=1$.

For the same reason, the transmission coefficient T also posseses these two kinds of symmetries. In the three-dimensional plots Figs. 3, 5, 7, and 8, we can find that there is a symmetric plane $(\Phi/\Phi_0=0.5,E)$ and two symmetric centers $(\Phi/\Phi_0=0.25,E=0)$ and $(\Phi/\Phi_0=0.75,E=0)$. The symmetric centers are most clearly displayed in Fig. 8, which is a three-dimensional plot for the second-generation SGL with two exits. If we compare the generalized eigenequation (5) with the eigenenergy equation (10), we can see that in the matrix M of Eq. (5) the matrix elements related with flux Φ are exactly the same as those of the eigenenergy equation (10). Therefore, they have the same dependence on the flux Φ. For a better view, in Figs. 4 and 6 we show some T-E cross sections of the three-dimensional T-Φ-E plots, which show that the pictures of $\Phi/\Phi_0=0.4$ and 0.6 are exactly the same, and those of $\Phi/\Phi_0=0.4$ and 0.1 are "antisymmetric," i.e., $T(\Phi/\Phi_0,E)=T(0.5-\Phi/\Phi_0,-E)$. Therefore, the transmission coefficient T is symmetric for $\pm E$ in the $\Phi/\Phi_0=0.25$ case. This point is clearly shown in the two-dimensional plots Figs. 4 and 6. These similarities also originate from the same relationship to flux Φ for both of the matrix equations (5) and (10).

Another interesting phenomenon displayed in the figures is that the single-exit SGL shows more complicated transmission behavior than the two-exit systems, i.e., in the former the transmission spectrum contains more peaks, valleys, and bigger fluctuation. An intuitive explanation for this phenomenon could be that from Fig. 2(b) we can see that the two exits in the open SGL are symmetric, both of which directly connect with the entry site by a straight lead, which serves as a direct "transport channel." This means that for the two-exit systems the multiscattering effect and the quantum-coherent effect of structure are weaker compared with the single-exit systems.

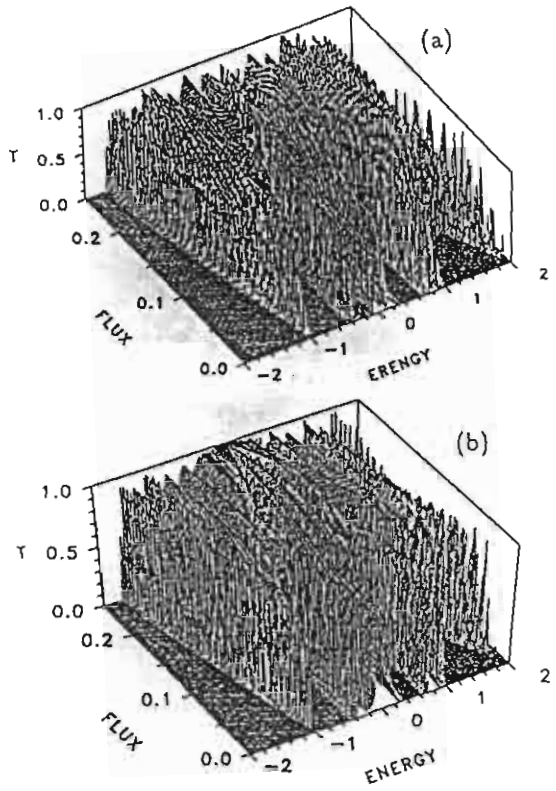

FIG. 11. Transmission coefficient T as a function of magnetic flux Φ and incident electron energy E for fourth-generation Sierpinski lattice. For the sake of clear visualization only a quarter of a period in flux Φ is shown. (a) Single-exit case. (b) Two-exit case.

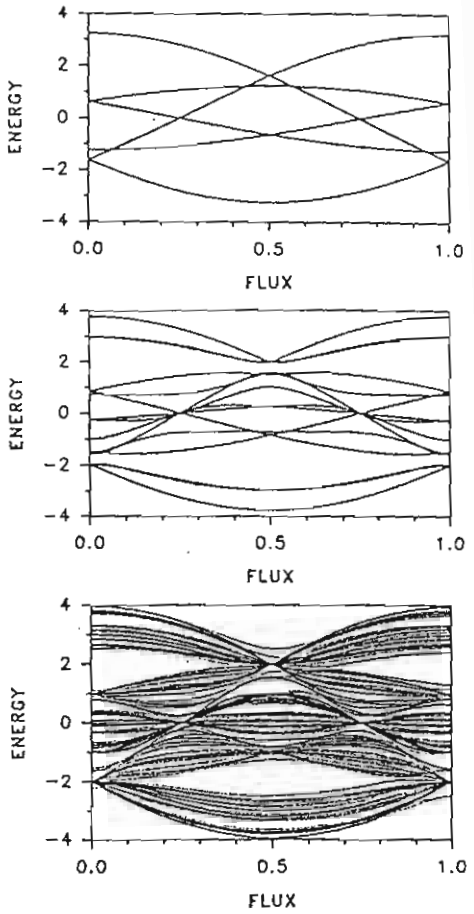

FIG. 12. Energy spectrum of isolated Sierpinski lattice as a function of magnetic flux Φ. From upper to bottom, they correspond to the first-, second-, and fourth-generation Shierpinski lattices, respectively. Readers should notice the symmetries of the spectrum to $\Phi/\Phi_0=0.5$ and 0.25.

In Figs. 6 and 9 we show the total and individual transmission coefficients T, T_1, T_2 for the first- and second-generation SGL with two exits. We can see the variation of the transmission coefficients T_1 and T_2 with the change of the magnetic flux Φ. Due to the modulation of the magnetic field, the T_1 and T_2 behaviors are different except in some special cases, such as $\Phi/\Phi_0=0$ and 0.5. Generally they periodically exchange the "position" following the variance of the flux Φ. This behavior comes from the fact that the two exits are symmetric in the structure of the SGL, therefore in the modulation of the magnetic field the T_1 and T_2 have a phase difference.

IV. BRIEF SUMMARY

We have introduced the generalized eigenfunction method (GEM), which is a very efficient and powerful approach to studying the electronic transport problems of aperiodic systems. By the use of the GEM we have studied the transport properties of open Sierpinski gasket lattices (SGL) coupled to two electron reservoirs via ideal leads. We have investigated the electronic transport properties of an open SGL up to its fourth-generation systems containing site number $N=123$. The main purpose of this paper is to investigate the behavior of the transmission coefficient T as the incident electron energy E and the magnetic flux Φ, which penetrates the elementary triangles of the SGL, are varied. The detailed numerical results are given in three-dimensional plots of transmission coefficient T against electron energy E and flux Φ, and in which the two-dimensional cross sections are T versus E. It is found that following the enlargement of the SGL, the transmission coefficient T fluctuates more and more, there are more and more resonant peaks, low-transmission valleys, and more and bigger antiresonant states ($T=0$) regions. In the transmission behaviors there are two kinds of symmetries to flux Φ. In the three-dimensional T-E-Φ plots, the transmission coefficient T has a symmetric plane ($\Phi/\Phi_0=0.5,E$) and two symmetric certers: ($\Phi/\Phi_0=0.25,E=0$) and ($\Phi/\Phi_0=0.75,E=0$). The numerical results show also that the transmission behavior of single-exit SGL systems is much more complicated than that of the two exit systems, because in the former there are direct "transport channels." It is different from the open ring systems now the electronic energies of the resonant states do not coincide with the eigenenergies of the isolated Sierpinski gasket systems. It means that the transport properties of the fractal systems are more complicated than those of the slab

systems[13,14] and ring systems.[18] The above results increase our understanding of the transport properties of fractal systems. In the present paper, as an example, we only discussed the SG, which is a simple fractal gasket derived from the Pascal triangle modulo 2, but it is well known that other strictly self-similar gaskets can be derived from Pascal triangle modulo n when n is prime, and even for a nonprime n there also exists self-similarity in the asymptotic sense.[29,30] For these fractal structures, determining what kind of universal property there is in the electronic transport problem would be a very interesting problem, and worth studying.

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On the Specific Heat of the Cubic Quasicrystals

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ABSTRACT Based on the linear elasticity theory of the cubic quasicrystals, we have derived the equations of wave propagating in the cubic quasicrystals and the analytical expression of the phase velocity of wave propagation. Moreover, we extend the Debye hypothesis of continuous elastic medium to study the specific heat of the cubic quasicrystals, for which we obtain an analytic expression of the specific heat as well as an approach to calculate the Debye temperature Θ_D.

KEYWORDS: specific heat, elasticity wave, quasicrystal.

INTRODUCTION

Since the discovery of the icosahedral quasicrystal in Al-Mn alloys, the quasicrystals with noncrystallographic symmetry, such as decagonal, dodecagonal and octagonal phases have been extensively studied.[1-4] For resent years in the process of the rapid solidified $V_6Ni_{16}Si_7$ alloy, Feng *et al*[5-6] discovered a kind of quasicrystal with cubic symmetry, which has been a new subject in the field of quasicrystals. Wang *et al*[7] have discussed the projection description of the cubic quasicrystals and Yang *et al*[8] have studied their linear elasticity theory. There are still many physical properties of the cubic quasicrystals have not been studied yet. For example, one of the important physical properties, the specific heat of cubic quasicrystals has not been studied. It is well-known that for the general quasicrystals it is impossible to obtain an analytical solution of lattice vibration properties. Therefore it is impossible to get an analytic result for the physical properties related to the quasicrystal-lattice dynamics. Due to the special structure of the cubic quasicrystals, we can obtain some analytical results on its lattice dynamics. In the present article we will report our study on the specific heat of cubic quasicrystals. We have first derived the equation of wave propagation in the cubic quasicrystals and then obtained the specific heat expression of the cubic quasicrystals. It is well-known that the calculation of the specific heat for both of the crystals and quasicrystals has to base on the knowledge of their lattice vibration modes. In order to simplify the calculation, Debye[9] assumed that the lattice wave of the solid is an elastic wave of continuous medium. Based on this hypothesis he successfully obtained the specific heat formulas and explained the experimental phenomenon that the specific heat of crystals decrease by T^3 at low temperature. In this paper, following the Debye hypothesis we will extend the continuous medium model to the cubic quasicrystals, in which the contributions of the phonons, phasons and their couplings on the specific heat are considered in the six-dimensional space but the wave propagaation still exists in the physical spaee.[5-8] By this generalized Debye hypothesis we first derive the wave equations to obtain the wave velocity expression, then we derive the analytical expression of specific heat for the cubic quasicrystals and provide a set of formulas to calculate the Debye temperature Θ_D. This paper is organized as follows: In Section II based on the linear elasticity theory we derive the wave propagation equation and phase velocities for the cubic quasicrystals. In Section III, based on the results of Section II, we derive the formulas to calculate the specific heat of the cubic quasicrystals. The Section IV is a brief conclusion. Because up to now there is no related experiment dates reported yet, therefore in this article we only present the theoretical results.

LINEAR ELASTICITY THEORY AND WAVE PROPAGATION EQUATION OF THE CUBIC QUASICRYSTALS

According to the result of Wang *et al*[7], the cubic quasicrystals can be obtained by projecting a six-dimensional periodic structure onto a three-dimensional physical subspace. Letting $\vec{\xi}$ be a

displacement vector in the six-dimensional space, u and w be the components of $\vec{\xi}$ in the parallel subspace (*ie*, physical subspace V_E) and perpendicular subspace (ie, complementary subspace V_I), respectively, then we have

$$\vec{\xi} = \mathrm{u} + \mathrm{w}. \qquad (1)$$

For the cubic quasicrystals which possess the crystallographic point-group symmetry, physical-property tensors in V_E and V_I can be transformed under the same irreducible representation. Therefore, they will induce the same elastic behavior in that two subspaces. If u_1, u_2, u_3 stand for the displacement components of the phonon field u, and w_1, w_2, w_3 for the displacement components of the phason field w along main-axis x_1, x_2, x_3, respectively, then we have

$$u_i = u_i(x_1, x_2, x_3; t)\ (i = 1, 2, 3);$$
$$w_i = w_i(x_1, x_2, x_3; t)\ (i = 1, 2, 3). \qquad (2)$$

According to the linear elasticity theory of the cubic quasicrystals developed by Yang *et al*[8], the stress-strain relations become

$$\begin{aligned}
T_{11} &= C_{11}E_{11} + C_{12}E_{22} + C_{12}E_{33} + R_1F_{11} + R_2F_{22} + R_2F_{33}\\
T_{22} &= C_{12}E_{11} + C_{11}E_{22} + C_{12}E_{33} + R_2F_{11} + R_1F_{22} + R_2F_{33}\\
T_{33} &= C_{12}E_{11} + C_{12}E_{22} + C_{11}E_{33} + R_2F_{11} + R_2F_{22} + R_1F_{33}\\
T_{23} &= 2C_{44}E_{23} + 2R_3F_{23} = T_{32}\\
T_{31} &= 2C_{44}E_{31} + 2R_3F_{31} = T_{13}\\
T_{21} &= 2C_{44}E_{12} + 2R_3F_{12} = T_{12}\\
H_{11} &= R_1E_{11} + R_2E_{22} + R_2E_{33} + K_{11}F_{11} + K_{12}F_{22} + K_{12}F_{33}\\
H_{22} &= R_2E_{11} + R_1E_{22} + R_2E_{33} + K_{12}F_{11} + K_{11}F_{22} + K_{12}F_{33}\\
H_{33} &= R_2E_{11} + R_2E_{22} + R_1E_{33} + K_{12}F_{12} + K_{12}F_{22} + K_{11}F_{33}\\
H_{23} &= 2R_3E_{23} + 2K_{44}F_{23} = H_{32}\\
H_{31} &= 2R_3E_{31} + 2K_{44}F_{31} = H_{13}\\
H_{12} &= 2R_3E_{12} + 2K_{44}F_{12} = H_{21} \qquad (3)
\end{aligned}$$

where E_{ij} are the strain components associated with phonon field u, F_{ij} the strain components associated with phason field w and

$$E_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \quad F_{ij} = \frac{1}{2}\left(\frac{\partial w_i}{\partial x_j} + \frac{\partial w_j}{\partial x_i}\right); \qquad (4)$$

T_{ij} are the stress components similar to those in conventional crystals, H_{ij} the stress components due to the existence of the phason field, C_{ij} the elastic constants of the phonon field, K_{ij} the elastic constants of the phason field, and R_i, the phonon-phason coupling elastic constants. The corresponding equations of mass-point vibration are

$$\begin{aligned}
\rho\frac{\partial^2 u_1}{\partial t^2} &= \frac{\partial T_{11}}{\partial x_1} + \frac{\partial T_{12}}{\partial x_2} + \frac{\partial T_{13}}{\partial x_3}\\
\rho\frac{\partial^2 u_2}{\partial t^2} &= \frac{\partial T_{21}}{\partial x_1} + \frac{\partial T_{22}}{\partial x_2} + \frac{\partial T_{23}}{\partial x_3}\\
\rho\frac{\partial^2 u_3}{\partial t^2} &= \frac{\partial T_{31}}{\partial x_1} + \frac{\partial T_{32}}{\partial x_2} + \frac{\partial T_{33}}{\partial x_3}\\
\rho\frac{\partial^2 w_1}{\partial t^2} &= \frac{\partial H_{11}}{\partial x_1} + \frac{\partial H_{12}}{\partial x_2} + \frac{\partial H_{13}}{\partial x_3}\\
\rho\frac{\partial^2 w_2}{\partial t^2} &= \frac{\partial H_{21}}{\partial x_1} + \frac{\partial H_{22}}{\partial x_2} + \frac{\partial H_{23}}{\partial x_3}\\
\rho\frac{\partial^2 w_3}{\partial t^2} &= \frac{\partial H_{31}}{\partial x_1} + \frac{\partial H_{32}}{\partial x_2} + \frac{\partial H_{33}}{\partial x_3} \qquad (5)
\end{aligned}$$

where ρ is the mass density of the quasicrystals. Because a cubic quasicrystal is an anisotropic crystal with nine independent elastic constants, the propagation of vibration varies with the polarization direction. In the following we first discuss the wave propagation in the direction $\wp$ of the physical space. Let *l*, *m*, *n* stand for the direction-cosines of $\wp$, we can rewrite the Eq (4) as follows:

$$\begin{aligned}
&E_{11} = l\frac{\partial u_1}{\partial \wp}, E_{22} = m\frac{\partial u_2}{\partial \wp}, E_{33} = n\frac{\partial u_3}{\partial \wp}, E_{23} = \frac{1}{2}\left(m\frac{\partial u_2}{\partial \wp} + n\frac{\partial u_3}{\partial \wp}\right),\\
&E_{13} = \frac{1}{2}\left(n\frac{\partial u_1}{\partial \wp} + l\frac{\partial u_3}{\partial \wp}\right), E_{23} = \frac{1}{2}\left(l\frac{\partial u_2}{\partial \wp} + m\frac{\partial u_1}{\partial \wp}\right),\\
&F_{11} = l\frac{\partial w_1}{\partial \wp}, F_{22} = m\frac{\partial w_2}{\partial \wp}, F_{33} = n\frac{\partial w_3}{\partial \wp}, F_{23} = \frac{1}{2}\left(m\frac{\partial w_2}{\partial \wp} + n\frac{\partial w_3}{\partial \wp}\right),\\
&F_{13} = \frac{1}{2}\left(n\frac{\partial w_1}{\partial \wp} + l\frac{\partial w_3}{\partial \wp}\right), F_{21} = \frac{1}{2}\left(l\frac{\partial w_2}{\partial \wp} + m\frac{\partial w_1}{\partial \wp}\right). \qquad (6)
\end{aligned}$$

Substituting Eq (6) into Eq (3), then into Eq (5) again, we can obtain

$$\begin{aligned}
\rho\frac{\partial^2 u_1}{\partial t^2} &= \Gamma_{11}\frac{\partial^2 u_1}{\partial \wp^2} + \Gamma_{12}\frac{\partial^2 u_2}{\partial \wp^2} + \Gamma_{13}\frac{\partial^2 u_3}{\partial \wp^2} + \Gamma_{14}\frac{\partial^2 w_1}{\partial \wp^2} + \Gamma_{15}\frac{\partial^2 w_2}{\partial \wp^2} + \Gamma_{16}\frac{\partial^2 w_3}{\partial \wp^2}\\
\rho\frac{\partial^2 u_2}{\partial t^2} &= \Gamma_{21}\frac{\partial^2 u_1}{\partial \wp^2} + \Gamma_{22}\frac{\partial^2 u_2}{\partial \wp^2} + \Gamma_{23}\frac{\partial^2 u_3}{\partial \wp^2} + \Gamma_{24}\frac{\partial^2 w_1}{\partial \wp^2} + \Gamma_{25}\frac{\partial^2 w_2}{\partial \wp^2} + \Gamma_{26}\frac{\partial^2 w_3}{\partial \wp^2}\\
\rho\frac{\partial^2 u_3}{\partial t^2} &= \Gamma_{31}\frac{\partial^2 u_1}{\partial \wp^2} + \Gamma_{32}\frac{\partial^2 u_2}{\partial \wp^2} + \Gamma_{33}\frac{\partial^2 u_3}{\partial \wp^2} + \Gamma_{34}\frac{\partial^2 w_1}{\partial \wp^2} + \Gamma_{35}\frac{\partial^2 w_2}{\partial \wp^2} + \Gamma_{36}\frac{\partial^2 w_3}{\partial \wp^2}\\
\rho\frac{\partial^2 w_1}{\partial t^2} &= \Gamma_{41}\frac{\partial^2 u_1}{\partial \wp^2} + \Gamma_{42}\frac{\partial^2 u_2}{\partial \wp^2} + \Gamma_{43}\frac{\partial^2 u_3}{\partial \wp^2} + \Gamma_{44}\frac{\partial^2 w_1}{\partial \wp^2} + \Gamma_{45}\frac{\partial^2 w_2}{\partial \wp^2} + \Gamma_{46}\frac{\partial^2 w_3}{\partial \wp^2} \qquad (7)
\end{aligned}$$

$$\rho\frac{\partial^2 w_1}{\partial t^2}=\Gamma_{51}\frac{\partial^2 u_1}{\partial \wp^2}+\Gamma_{52}\frac{\partial^2 u_2}{\partial \wp^2}+\Gamma_{53}\frac{\partial^2 u_3}{\partial \wp^2}+\Gamma_{54}\frac{\partial^2 w_1}{\partial \wp^2}+\Gamma_{55}\frac{\partial^2 w_2}{\partial \wp^2}+\Gamma_{56}\frac{\partial^2 w_3}{\partial \wp^2}$$

$$\rho\frac{\partial^2 w_2}{\partial t^2}=\Gamma_{61}\frac{\partial^2 u_1}{\partial \wp^2}+\Gamma_{62}\frac{\partial^2 u_2}{\partial \wp^2}+\Gamma_{63}\frac{\partial^2 u_3}{\partial \wp^2}+\Gamma_{64}\frac{\partial^2 w_1}{\partial \wp^2}+\Gamma_{65}\frac{\partial^2 w_2}{\partial \wp^2}+\Gamma_{66}\frac{\partial^2 w_3}{\partial \wp^2},$$

where

$$\begin{cases}\Gamma_{11}=C_{11}l^2+C_{44}(m^2+n^2) & \Gamma_{21}=C_{12}lm+C_{44}lm\\ \Gamma_{12}=C_{12}lm+C_{44}lm & \Gamma_{22}=C_{11}m^2+C_{44}(l^2+n^2)\\ \Gamma_{13}=C_{12}ln+C_{44}ln & \Gamma_{23}=C_{12}mn+C_{44}mn\\ \Gamma_{14}=R_1l^2+R_3(m^2+n^2) & \Gamma_{24}=R_2lm+R_3lm\\ \Gamma_{15}=R_2lm+R_3lm & \Gamma_{25}=R_1m^2+R_3(l^2+n^2)\\ \Gamma_{16}=R_2ln+R_3ln, & \Gamma_{26}=R_2mn+R_3mn,\end{cases} \quad (8)$$

$$\begin{cases}\Gamma_{31}=C_{12}ln+C_{44}ln & \Gamma_{41}=R_1l^2+R_3(m^2+n^2)\\ \Gamma_{32}=C_{12}mn+C_{44}mn & \Gamma_{42}=R_2lm+R_3lm\\ \Gamma_{33}=C_{12}n^2+C_{44}(l^2+m^2) & \Gamma_{43}=R_2ln+R_3ln\\ \Gamma_{34}=R_2ln+R_3ln & \Gamma_{44}=K_{11}l^2+K_{44}(m^2+n^2)\\ \Gamma_{35}=R_2mn+R_3mn & \Gamma_{45}=K_{12}lm+K_{44}lm\\ \Gamma_{36}=R_1n^2+R_3(l^2+m^2); & \Gamma_{46}=R_{12}mn+R_{44}mn,\end{cases} \quad (9)$$

$$\begin{cases}\Gamma_{51}=R_2lm+R_3lm & \Gamma_{61}=R_2ln+R_3ln\\ \Gamma_{52}=R_1m^2+R_3(l^2+n^2) & \Gamma_{62}=R_2mn+R_3mn\\ \Gamma_{53}=R_2mn+R_3mn & \Gamma_{63}=R_1n^2+R_3(l^2+m^2)\\ \Gamma_{54}=K_{12}lm+K_{44}lm & \Gamma_{64}=K_{12}ln+K_{44}ln\\ \Gamma_{55}=K_{11}m^2+K_{44}(l^2+n^2) & \Gamma_{65}=K_{12}mn+K_{44}mn\\ \Gamma_{56}=K_{12}mn+K_{44}mn & \Gamma_{66}=K_{11}n^2+K_{44}(l^2+m^2).\end{cases} \quad (10)$$

Let $\vec{\xi}$ stand for elastic displacement vector related to the wave propagation along $\wp$ direction, and p, q, r, p', q', r' for its direction-cosines in the six-dimensional space, then

$$u_1=p\xi,\ u_2=q\xi,\ u_3=r\xi,\ w_1=p'\xi,\ w_2=q\xi,\ w_3=r\xi,$$
$$\xi=pu_1+qu_2+ru_3+p'w_1+q'w_2+r'w_3, \quad (11)$$

where ξ is the length of $\vec{\xi}$. Substituting Eq (11) into Eq (7), we obtain the following wave equation

$$p\frac{\partial^2\xi}{\partial t^2}=C^*\frac{\partial^2\xi}{\partial \wp^2}, \quad (12)$$

which implies that the phase velocity $v=\sqrt{C^*/p}$, C^* is the effective elasticity coefficient, and satisfies the following equations:

$$\begin{aligned}
&p\Gamma_{11}+q\Gamma_{12}+r\Gamma_{13}+p'\Gamma_{14}+q'\Gamma_{15}+r'_{16}\Gamma_{16}=pC^*\\
&p\Gamma_{21}+q\Gamma_{22}+r\Gamma_{23}+p'\Gamma_{24}+q'\Gamma_{25}+r'_{26}\Gamma_{26}=qC^*\\
&p\Gamma_{31}+q\Gamma_{32}+r\Gamma_{33}+p'\Gamma_{34}+q'\Gamma_{35}+r'_{36}\Gamma_{36}=rC^*\\
&p\Gamma_{41}+q\Gamma_{42}+r\Gamma_{43}+p'\Gamma_{44}+q'\Gamma_{45}+r'_{46}\Gamma_{46}=p'C^*\\
&p\Gamma_{51}+q\Gamma_{52}+r\Gamma_{53}+p'\Gamma_{54}+q'\Gamma_{55}+r'_{56}\Gamma_{56}=q'C^*\\
&p\Gamma_{61}+q\Gamma_{62}+r\Gamma_{63}+p'\Gamma_{64}+q'\Gamma_{65}+r'_{66}\Gamma_{66}=r'C^*.
\end{aligned} \quad (13)$$

Providing that the Eq (13) has a solution, then we have

$$\begin{vmatrix}
\Gamma_{11}-C^*\Gamma_{12} & \Gamma_{13} & \Gamma_{14} & \Gamma_{15} & \Gamma_{16}\\
\Gamma_{21} & \Gamma_{22}-C^* & \Gamma_{23} & \Gamma_{24} & \Gamma_{25} & \Gamma_{26}\\
\Gamma_{31}-C^*\Gamma_{32} & \Gamma_{33}-C^* & \Gamma_{34} & \Gamma_{35} & \Gamma_{36}\\
\Gamma_{41} & \Gamma_{42} & \Gamma_{43} & \Gamma_{44}-C^* & \Gamma_{45} & \Gamma_{46}\\
\Gamma_{51} & \Gamma_{52} & \Gamma_{53} & \Gamma_{54} & \Gamma_{55}-C^* & \Gamma_{56}\\
\Gamma_{61} & \Gamma_{62} & \Gamma_{63} & \Gamma_{64} & \Gamma_{65} & \Gamma_{66}-C^*
\end{vmatrix}=0. \quad (14)$$

Above Eq (14) is a secular-equation of effective elastic constants C^*. In principal, combining Eqs (8-10) we can solve the Eq (14) to obtain C^* and then calculate the phase-velocities of wave propagation along any direction. It is however very difficult to analytically solve the Eq (14) for all propagation direction. To simplify the calculation and obtain a possible analytical solution, we consider the wave propagating along the (100) direction of cubic quasicrystals in physical subspace. In this special cace Eq (14) reduces to

$$\begin{vmatrix}
C_{11}-C^* & 0 & 0 & R_1 & 0 & 0\\
0 & C_{44}-C^* & 0 & 0 & R_3 & 0\\
0 & 0 & C_{44}-C^* & 0 & 0 & R_3\\
R_1 & 0 & 0 & K_{11}-C^* & 0 & 0\\
0 & R_3 & 0 & 0 & K_{44}-C^* & 0\\
0 & 0 & R_3 & 0 & 0 & K_{44}-C^*
\end{vmatrix}=0. \quad (15)$$

The solutions of above equation are, respectively,

$$C_1^* = C_4^* = \tfrac{1}{2}(C_{11} + K_{11}) + \frac{2R_1^2}{\sqrt{(C_{11}-K_{11})^2 + 4R_1^2}}, \quad (16)$$

$$C_2^* = C_3^* = C_5^* = C_6^* = \tfrac{1}{2}(C_{44} + K_{44}) + \frac{2R_3^2}{\sqrt{(C_{44}-K_{44})^2 + 4R_3^2}},$$

then the six velocities, $v_i (i = 1, \ldots 6)$, of wave propagating along the (100) direction of the cubic quasicrystals in physical-subspace have the following expressions:

$$v_1 = v_4 = \sqrt{\frac{\tfrac{1}{2}(C_{11} + K_{11}) + \frac{2R_1^2}{\sqrt{(C_{11}-K_{11})^2 + 4R_1^2}}}{\rho}}$$

$$v_2 = v_3 = v_5 = v_6 = \sqrt{\frac{\tfrac{1}{2}(C_{44} + K_{44}) + \frac{2R_3^2}{\sqrt{(C_{44}-K_{44})^2 + 4R_3^2}}}{\rho}}. \quad (17)$$

From above formulas we can see that Eq. (17) contains only four parameters C_{11}, K_{11}, R_1 and R_3. If we consider other propagation direction, says, to calculate the phase velocities of wave propagating along the (111) direction, then from Eq. (14) we will see that the velocity expression would involve nine independent elastic constants of the cubic quasicrystals. Obtaining an analytic solution is therefore very difficult. For these more general cases ones can only expect to have a numerical solution.

Specific Heat of the Cubic Quasicrystals

After obtaining the above velocity expressions we now can evaluate the specific heat of the cubic quasicrystals by extending the Debye hypothesis to the studied systems. Debye[9] considered the crystals as a continuous elastic medium to propagate the waves of elastic vibration. Under this hypothesis he calculated the specific heat of ideal crystals, which was in good agreement with the experimental results at low temperature. We will now try to extend the Debye hypotheses to the cubic quasicrystals, i.e., we also consider the cubic quasicrystal as a continuous elastic medium. Noting that the phason do not form new degrees of freedom, the total number of freedom degrees remains three times the number of atoms contained in the cubic quasicrystal. Therefore, there are 3N independent harmonic vibration modes, where N is the number of atoms in the cubic quasicrystal. Denoting ω for the atom vibration circle-frequency and $g(\omega)$ for the frequency distribution function, then $g(\omega)d\omega$ is the number of the harmonic vibration modes between ω and $\omega + d\omega$, and we have

$$\int_0^\infty g(\omega)d\omega = 3N. \quad (18)$$

For the cubic quasicrystals containing phonon as well as phason by the Debye hypothesis we have

$$g(\omega)d\omega = B\omega^2 d\omega, \quad (19)$$

where

$$B = \frac{V}{2\pi^2}\left(\frac{1}{v_1^3} + \frac{1}{v_2^3} + \frac{1}{v_3^3} + \frac{1}{v_4^3} + \frac{1}{v_5^3} + \frac{1}{v_6^3}\right), \quad (20)$$

and V represents the volume of the cubic quasicrystals, $v_i (i = 1, \ldots, 6)$ are defined by Eq (17).

Considering that the total number of freedom degrees should be finite, so there is a maximum frequency w_D, then Eq (18) can be rewritten as

$$\int_0^{\omega_D} g(\omega)d\omega = 3N. \quad (21)$$

Substituting Eq (19) into the above formula and because the phase velocities v_i, $i = 1,2, \ldots 6$ are independent of the frequency, so we easily obtain

$$\omega_D^3 = 9N/B. \quad (22)$$

If we introduce an effective average energy , then the total energy reads

$$E = E_0 + \sum_{\omega} \bar{\varepsilon}(\omega) = E_0 + \int_0^{\omega_D} \bar{\varepsilon}(\omega) g(\omega) d\omega, \quad (23)$$

where E_0 is a constant and

$$\bar{\varepsilon} = \frac{\hbar\omega}{e^{\hbar\omega/kT} - 1}, \quad (24)$$

where k is the Boltzmann constant, T is the absolute temperature, respectively. According to the definition of specific heat,

$$C_V = \left(\frac{\partial E}{\partial T}\right)_V. \quad (25)$$

Using Eqs (22-24) we obtain

$$C_V = B\int_0^{\omega_D} (\frac{\hbar\omega}{kT})^2 \frac{e^{\hbar\omega/kT} k\omega^2 d\omega}{(e^{\hbar\omega/kT}-1)^2}, \qquad (26)$$

where B is given by Eq. (20). If we introduce two new parameters x and y as following:

$$y = \frac{\hbar\omega}{kT}, \quad x = \frac{\hbar\omega_D}{kT} = \frac{\Theta_D}{T}, \qquad (27)$$

where Θ_D is the generalized Debye characteristic temperature for the cubic quasicrystals, and evaluated as

$$\Theta_D = \hbar\omega_D/k = \frac{\hbar}{k}(\frac{9N}{B})^{1/3} = \frac{\hbar}{k}(\frac{18N\pi^2}{B})^{1/3}\frac{1}{\chi^{1/3}} \qquad (28)$$

with

$$\chi = (\frac{1}{v_1^3}+\frac{1}{v_2^3}+\frac{1}{v_3^3}+\frac{1}{v_4^3}+\frac{1}{v_5^3}+\frac{1}{v_6^3}), \qquad (29)$$

then the Eq. (26) can be rewritten as

$$C_V = Bk\int_0^x (kT/\hbar)^3 \frac{y^4 e^y}{(e^y-1)^2} dy$$

$$= \frac{9Nk}{x^3}\int_0^x \frac{y^4 e^y}{(e^y-1)^2} dy. \qquad (30)$$

Above Eq (30) is an analytic expression of specific heat for tbe cubic quasicrystals. It is also one of the main analytic results which we expect to obtain.

Conclusion

In this paper, we first obtained the wave propagation equation of the cubic quasicrystals. Based on this equation, we derived the formulas of wave velocities propagating in the cubic quasicrystals. By extending the Debye's continuous medium hypothesis for ideal crystals to the cubic quasicrystals, we obtained the analytic expresion of specific heat for the cubic quasicrystals and provided an approach to calculate the Debye temperature Θ_D. Formally the present specific heat and Debye temperature expressions for cubic quasicrystals are almost same as that of the ideal crystals, but the Θ_D contains the contributions of the phonons, the phasons, and the coupling between phonons and phasons. Thus, the present theoretical results on the specific heat of the cubic quasicrystals are an meaningful extension of the Debye theory for ideal crystals, and also only because the special geometric structure of the cubic quasicrystals we can obtain these interesting analytical results, for other kinds of quasicrystals we generally can not obtain such impact analytical solution. Ones can only expect a numerical result, but it is a heavy and tedious work.

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On the Fourier transform of the Diamond Kernel of Marcel Riesz

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Abstract

In this paper, the operator $\Diamond^k$ is introduced and named as the Diamond operator iterated k-times and is defined by $\Diamond^k = [(\partial^2/\partial x_1^2 + \partial^2/\partial x_2^2 + \cdots + \partial^2/\partial x_p^2)^2 - (\partial^2/\partial x_{p+1}^2 + \partial^2/\partial x_{p+2}^2 + \cdots + \partial^2/\partial x_{p+q}^2)^2]^k$, where n is the dimension of the Euclidean space $\mathbb{R}^n$, k is a nonnegative integer and $p+q=n$. The elementary solution of the operator $\Diamond^k$ is called the Diamond Kernel of Marcel Riesz. In this work we study the Fourier transform of the elementary solution and also the Fourier transform of their convolutions.

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Keywords: Diamond operator; Fourier transform; Kernel of Marcel Riesz; Dirac delta distributions; Tempered distribution

1. Introduction

Consider the equation

$$\Diamond^k u(x) = \delta, \tag{1}$$

where $\Diamond^k$ is the Diamond operator iterated k-times ($k = 0, 1, 2, \ldots$) with $\Diamond^0 u(x) = u(x)$ and is defined by

$$\Diamond^k = \left(\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \cdots + \frac{\partial^2}{\partial x_p^2} \right)^2 - \left(\frac{\partial^2}{\partial x_{p+1}^2} + \frac{\partial^2}{\partial x_{p+2}^2} + \cdots + \frac{\partial^2}{\partial x_{p+q}^2} \right)^2 \right)^k, \tag{2}$$

where $p+q=n$, the dimension of the Euclidean space $\mathbb{R}^n$ and $u(x)$ is the generalized function, $x = (x_1, x_2, \ldots x_n) \in \mathbb{R}^n$ and δ is the Dirac-delta distribution.

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Kananthai ([1], Theorem 1.3) has shown that the solution of convolution form $u(x) = (-1)^k S_{2k}(x) * R_{2k}(x)$ is an unique elementary solution of Eq. (1) where $S_{2k}(x)$ and $R_{2k}(x)$ are defined by Eqs. (4) and (6), respectively, with $\alpha = 2k$. Now $(-1)^k S_{2k}(x) * R_{2k}(x)$ is a generalized function, see [1], and is called the Diamond Kernel of Marcel Riesz. In this paper we study the Fourier transform of $(-1)^k S_{2k}(x) * R_{2k}(x)$ and the Fourier transform of $[(-1)^k S_{2k}(x) * R_{2k}(x)] * [(-1)^m S_{2m}(x) * R_{2m}(x)]$ where k and m are nonnegative integers.

2. Preliminaries

Definition 2.1. Let $E(x)$ be a function defined by

$$E(x) = \frac{|x|^{2-n}}{(2-n)\omega_n}, \tag{3}$$

where $x = (x_1, \ldots, x_n) \in \mathbb{R}^n$, $|x| = (x_1^2 + \cdots + x_n^2)^{1/2}$ and $\omega_n = (2\pi^{n/2})/\Gamma(n/2)$ is a surface area of the unit sphere.

It is well known that $E(x)$ is an elementary solution of the Laplace operator Δ, that is $\Delta E(x) = \delta$ where $\Delta = \sum_{i=1}^{n} (\partial^2/\partial x_i^2)$ and δ is the Dirac-delta distribution.

Definition 2.2. Let $S_\alpha(x)$ be a function defined by

$$S_\alpha(x) = 2^{-\alpha}\pi^{-n/2}\Gamma\left(\frac{n-\alpha}{2}\right)\frac{|x|^{\alpha-n}}{\Gamma\left(\frac{\alpha}{2}\right)}, \tag{4}$$

where α is a complex parameter, $|x| = (x_1^2 + \cdots + x_n^2)^{1/2}$, $x = (x_1, \ldots, x_n) \in \mathbb{R}^n$.

$S_\alpha(x)$ is called the Elliptic Kernel of Marcel Riesz. Now $S_\alpha(x)$ is an ordinary function for $\mathrm{Re}(\alpha) \geqslant n$ and is a distribution of α for $\mathrm{Re}(\alpha) < n$.

From Eqs. (3) and (4) we obtain

$$E(x) = -S_2(x). \tag{5}$$

Definition 2.3. Let $x = (x_1, \ldots, x_n)$ be a point in $\mathbb{R}^n$ and write

$$V = x_1^2 + x_2^2 + \cdots + x_p^2 - x_{p+1}^2 - x_{p+2}^2 - \cdots - x_{p+q}^2,$$

where $p + q = n$. Define $\Gamma_+ = \{x \in \mathbb{R}^n\colon x_1 > 0 \text{ and } V > 0\}$ designating the interior of the forward cone and denote $\bar{\Gamma}_+$ by its closure and the following function introduced by Nozaki ([2], p. 72),

$$R_\alpha(x) = \begin{cases} \dfrac{V^{(\alpha-n)/2}}{K_n(\alpha)}, & \text{if } x \in \Gamma_+, \\ 0, & \text{if } x \notin \Gamma_+. \end{cases} \tag{6}$$

Here $R_\alpha(x)$ is called the ultra-hyperbolic kernel of Marcel Riesz and α is a complex parameter and n is the dimension of the space $\mathbb{R}^n$.

The constant $K_n(\alpha)$ is defined by

$$K_n(\alpha) = \frac{\pi^{(n-1)/2}\Gamma\left(\frac{2+\alpha-n}{2}\right)\Gamma\left(\frac{1-\alpha}{2}\right)\Gamma(\alpha)}{\Gamma\left(\frac{2+\alpha-\rho}{2}\right)\Gamma\left(\frac{\rho-\alpha}{2}\right)}.$$

Here $R_\alpha(x)$ is an ordinary function if $\mathrm{Re}(\alpha) \geqslant n$ and is a distribution of α if $\mathrm{Re}(\alpha) < n$.

Let $\mathrm{supp}\, R_\alpha(x) \subset \bar{\Gamma}_+$ where $\mathrm{supp}\, R_\alpha(x)$ denote the support of $R_\alpha(x)$.

Definition 2.4. Let f be a continuous function, the Fourier transform of f denoted by

$$\mathscr{F}f = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-i\xi x}\, dx, \tag{7}$$

where $x = (x_1, \ldots, x_n) \in \mathbb{R}^n, \xi = (\xi_1, \ldots, \xi_n) \in \mathbb{R}^n$ and $\xi x = \xi_1 x_1 + \xi_2 x_2 + \cdots + \xi_n x_n$. Sometimes we write $\mathscr{F}f(x) \equiv \hat{f}(\xi)$. By Eq. (7), we can define the inverse of the Fourier transform of $\hat{f}(\xi)$ by

$$f(x) = \mathscr{F}^{-1}\hat{f}(\xi) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{i\xi x}\hat{f}(\xi)\, d\xi. \tag{8}$$

If f is a distribution with compact supports by [3], Theorem 7.4-3, p. 187 Eq. (7) can be written as

$$\mathscr{F}f = \frac{1}{(2\pi)^{n/2}} \langle f(x), e^{-i\xi x} \rangle. \tag{9}$$

Lemma 2.1. *The functions $S_\alpha(x)$ and $R_\alpha(x)$ defined by Eqs. (4) and (6), respectively, for $\mathrm{Re}(\alpha) < n$ are homogeneous distributions of order $\alpha - n$.*

Proof. Since $R_\alpha(x)$ and $S_\alpha(x)$ satisfy the Euler equation, that is

$$(\alpha - n)R_\alpha(x) = \sum_{i=1}^{n} x_i \frac{\partial}{\partial x_i} R_\alpha(x) \text{ and } (\alpha - n)S_\alpha(x) = \sum_{i=1}^{n} x_i \frac{\partial}{\partial x_i} S_\alpha(x),$$

we have that $R_\alpha(x)$ and $S_\alpha(x)$ are homogeneous distributions of order $\alpha - n$.

Donoghue ([4], pp. 154 and 155) has proved that every homogeneous distribution is a tempered distribution.

That completes the proof.

Lemma 2.2 (The convolution of tempered distributions). *The convolution $S_\alpha(x) * R_\alpha(x)$ exists and is a tempered distribution.*

Proof. Choose supp $R_\alpha(x) = K \subset \bar{\Gamma}_+$ where K is a compact set. Then $R_\alpha(x)$ is a tempered distribution with compact support and by [3], pp. 156–159 $S_\alpha(x) * R_\alpha(x)$ exists and is a tempered distribution.

Lemma 2.3. *Given the equation* $\Diamond^k u(x) = \delta$ *where the operator* $\Diamond^k$ *is defined by Eq. (2),* $x = (x_1, \ldots, x_n) \in \mathbb{R}^n$, k *is a nonnegative integer and* δ *is the Dirac-delta distribution, then* $u(x) = (-1)^k S_{2k}(x) * R_{2k}(x)$ *is the unique elementary solution of the equation where* $S_{2k}(x)$ *and* $R_{2k}(x)$ *are defined by Eqs. (4) and (6), respectively, with* $\alpha = 2k$.

Proof. By Lemma 2.2, for $\alpha = 2k$, the distribution $(-1)^k S_{2k}(x) * R_{2k}(x)$ exists and is a tempered distribution.

Now the distribution $(-1)^k S_{2k}(x)$ is obtained by the convolution

$$\underbrace{E(x) * E(x) * \cdots * E(x)}_{k\text{-times}} = \underbrace{(-S_2(x)) * (-S_2(x)) * \cdots * (-S_2(x))}_{k\text{-times}},$$

where $E(x)$ is defined by Eq. (3) and by Eq. (5).

Kananthai ([5], Lemma 2.5) has shown that

$$\underbrace{-S_2(x) * (-S_2(x)) * \cdots * (-S_2(x))}_{k\text{-times}} = (-1)^k S_{2k}(x)$$

is an elementary solution of the Laplace operator Δ^k iterated k-times. By Eq. (2), $\Diamond^k$ can be written as

$$\Diamond^k = \Box^k \Delta^k, \tag{10}$$

where

$$\Box^k = \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \cdots + \frac{\partial^2}{\partial x_p^2} - \frac{\partial^2}{\partial x_{p+1}^2} - \cdots - \frac{\partial^2}{\partial_{p+q}^2} \right)^k$$

and

$$\Delta^k = \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \cdots + \frac{\partial^2}{\partial x_n^2} \right)^k, \quad p + q = n.$$

By [1], Theorem 3.1 $u(x) = (-1)^k S_{2k}(x) * R_{2k}(x)$ is the unique elementary solution of the operator $\Diamond^k$ as required.

Lemma 2.4 (The Fourier transform of $\Diamond^k \delta$).

$$\mathcal{F} \Diamond^k \delta = \frac{1}{(2\pi)^{n/2}} \left((\xi_1^2 + \xi_2^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \xi_{p+2}^2 + \cdots + \xi_{p+q}^2)^2 \right)^k,$$

where $\mathcal{F}$ is the Fourier transform defined by Eq. (7) and if the norm of ξ is given by $\|\xi\| = (\xi_1^2 + \xi_2^2 + \cdots + \xi_n^2)^{1/2}$ *then*

$$|\mathcal{F}\Diamond^k\delta| \leqslant \frac{1}{(2\pi)^{n/2}}\|\xi\|^{4k} \tag{11}$$

that is $\mathcal{F}\Diamond^k\delta$ is bounded and continuous on the space S' of the tempered distribution. Moreover, by Eq. (8)

$$\Diamond^k\delta = \mathcal{F}^{-1}\frac{1}{(2\pi)^{n/2}}\left((\xi_1^2 + \xi_2^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \xi_{p+2}^2 + \cdots + \xi_{p+q}^2)^2\right)^k.$$

Proof. By Eq. (9)

$$\begin{aligned}
\mathcal{F}\Diamond^k\delta &= \frac{1}{(2\pi)^{n/2}}\langle\Diamond^k\delta, e^{-i\xi x}\rangle \\
&= \frac{1}{(2\pi)^{n/2}}\langle\delta, \Diamond^k e^{-i\xi x}\rangle \\
&= \frac{1}{(2\pi)^{n/2}}\langle\delta, \Box^k\Delta^k e^{-i\xi x}\rangle \quad \text{by (10)} \\
&= \frac{1}{(2\pi)^{n/2}}\langle\delta, (-1)^k(\xi_1^2 + \xi_2^2 + \cdots + \xi_n^2)^k\Box^k e^{-i\xi x}\rangle \\
&= \frac{1}{(2\pi)^{n/2}}\langle\delta, (-1)^k(\xi_1^2 + \xi_2^2 + \cdots + \xi_n^2)^k(-1)^k \\
&\quad \times (\xi_1^2 + \xi_2^2 + \cdots + \xi_p^2 - \xi_{p+1}^2 - \xi_{p+2}^2 - \cdots - \xi_{p+2}^2)^k e^{-i\xi x}\rangle \\
&= \frac{1}{(2\pi)^{n/2}}(-1)^{2k}((\xi_1^2 + \cdots + \xi_n^2)^k \times (\xi_1^2 + \cdots + \xi_p^2 - \xi_{p+1}^2 - \cdots - \xi_{p+q}^2)^k \\
&= \frac{1}{(2\pi)^{n/2}}\left((\xi_1^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \cdots + \xi_{p+q}^2)^2\right)^k.
\end{aligned}$$

Now

$$\begin{aligned}
|\mathcal{F}\Diamond^k\delta| &= \frac{1}{(2\pi)^{n/2}}\left(|\xi_1^2 + \cdots + \xi_n^2||\xi_1^2 + \cdots + \xi_p^2 - \xi_{p+1}^2 - \cdots \xi_{p+q}^2|\right)^k \\
&\leqslant \frac{1}{(2\pi)^{n/2}}\left(|\xi_1^2 + \cdots + \xi_n^2|\right)^k \\
&= \frac{1}{(2\pi)^{n/2}}\|\xi\|^{4k},
\end{aligned}$$

where $\|\xi\| = (\xi_1^2 + \cdots + \xi_n^2)^{1/2}$, $\xi_i\ (i = 1, 2, \ldots, n) \in \mathbb{R}$. Hence we obtain Eq. (11) and $\mathcal{F}\Diamond^k\delta$ is bounded and continuous on the space S' of the tempered distribution.

Since $\mathcal{F}$ is 1–1 transformation from the space S' of the tempered distribution to the real space R, then by Eq. (8)

$$\Diamond^k\delta = \frac{1}{(2\pi)^{n/2}}\mathcal{F}^{-1}\left((\xi_1^2+\cdots+\xi_p^2)^2-(\xi_{p+1}^2+\cdots+\xi_{p+q}^2)^2\right)^k.$$

That completes the proof.

3. Main results

Theorem 3.1.

$$\mathcal{F}((-1)^kS_{2k}(x)*R_{2k}(x)) = \frac{1}{(2\pi)^{n/2}[(\xi_1^2+\cdots+\xi_p^2)^2-(\xi_{p+1}^2+\cdots+\xi_{p+q}^2)^2]^k}$$

and

$$|\mathcal{F}((-1)^kS_{2k}(x)*R_{2k}(x))| \leqslant \frac{1}{(2\pi)^{n/2}}M \text{ for a large } \xi_i\in R, \tag{12}$$

where M is a constant. That is $\mathcal{F}$ is bounded and continuous on the space S' of the tempered distributions.

Proof. By Lemma 2.3 $\Diamond^k((-1)^kS_{2k}(x)*R_{2k}(x)=\delta$ or $(\Diamond^k\delta)*[(-1)^kS_{2k}(x)*R_{2k}(x)]=\delta$.

Taking the Fourier transform on both sides, we obtain

$$\mathcal{F}((\Diamond^k\delta)*[(-1)^kS_{2k}(x)*R_{2k}(x)]) = \mathcal{F}\delta = \frac{1}{(2\pi)^{n/2}}.$$

By Eq. (9)

$$\frac{1}{(2\pi)^{n/2}}\langle(\Diamond^k\delta)*[(-1)^kS_{2k}(x)*R_{2k}(x)], e^{-i\xi x}\rangle = \frac{1}{(2\pi)^{n/2}}.$$

By the definition of convolution

$$\frac{1}{(2\pi)^{n/2}}\langle(\Diamond^k\delta),\langle[(-1)^kS_{2k}(r)*R_{2k}(r)], e^{-i\xi(x+r)}\rangle\rangle = \frac{1}{(2\pi)^{n/2}},$$

$$\frac{1}{(2\pi)^{n/2}}\langle[(-1)^kS_{2k}(r)*R_{2k}(r)], e^{-i\xi r}\rangle\langle(\Diamond^k\delta), e^{-i\xi x}\rangle = \frac{1}{(2\pi)^{n/2}},$$

$$\mathcal{F}([(-1)^kS_{2k}(r)*R_{2k}(r)])(2\pi)^{n/2}\mathcal{F}(\Diamond^k\delta) = \frac{1}{(2\pi)^{n/2}}.$$

By Lemma 2.4,

$$\mathcal{F}([(-1)^k S_{2k}(x) * R_{2k}(x)])((\xi_1^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \cdots + \xi_{p+q}^2)^2)^k = \frac{1}{(2\pi)^{n/2}}.$$

It follows that

$$\mathcal{F}([(-1)^k S_{2k}(x) * R_{2k}(x)]) = \frac{1}{(2\pi)^{n/2}[(\xi_1^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \cdots + \xi_{p+q}^2)^2]^k}.$$

Now

$$\frac{1}{[(\xi_1^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \cdots + \xi_{p+q}^2)^2]^k} = \frac{1}{(\xi_1^2 + \cdots + \xi_n^2)^k} \frac{1}{(\xi_1^2 + \cdots + \xi_p^2 - \xi_{p+1}^2 - \cdots - \xi_{p+q}^2)^k}. \tag{13}$$

Let $\xi = (\xi_1, \ldots, \xi_n) \in \Gamma_+$ with Γ_+ defined by Definition 2.3. Then $(\xi_1^2 + \cdots + \xi_p^2 - \xi_{p+1}^2 - \cdots - \xi_{p+q}^2) > 0$ and for a large ξ_i and a large k, the right-hand side of Eq. (13) tends to zero. It follows that it is bounded by a positive constant M say, that is we obtain Eq. (12) as required and also by Eq. (12) $\mathcal{F}$ is continuous on the space S' of the tempered distribution.

Theorem 3.2.

$$\begin{aligned}&\mathcal{F}([(-1)^k S_{2k}(x) * R_{2k}(x)] * [(-1)^m S_{2m}(x) * R_{2m}(x)])\\ &= (2\pi)^{n/2}\mathcal{F}([(-1)^k S_{2k}(x) * R_{2k}(x)]\mathcal{F}[(-1)^m S_{2m}(x) * R_{2m}(x)]\\ &= \frac{1}{(2\pi)^{n/2}} \frac{1}{[(\xi_1^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \cdots + \xi_{p+q}^2)^2]^{k+m}},\end{aligned}$$

where k and m are nonnegative integers and $\mathcal{F}$ is bounded and continuous on the space S' of the tempered distribution.

Proof. Since $R_{2k}(x)$ and $S_{2k}(x)$ are tempered distributions with compact supports, we have

$$\begin{aligned}&[(-1)^k S_{2k}(x) * R_{2k}(x)] * [(-1)^m S_{2m}(x) * R_{2m}(x)]\\ &= (-1)^{k+m}(S_{2k}(x) * S_{2m}(x)) * (R_{2k}(x) * R_{2m}(x))\\ &= (-1)^{k+m}(S_{2(k+m)}(x) * R_{2(k+m)}(x))\end{aligned}$$

by [3], pp. 156–159 and [2], Lemma 2.5. Taking the Fourier transform on both sides and using Theorem 3.1 we obtain

$$\begin{aligned}
&\mathcal{F}([(-1)^k S_{2k}(x) * R_{2k}(x)] * [(-1)^m S_{2m}(x) * R_{2m}(x)]) \\
&= \frac{1}{(2\pi)^{n/2}((\xi_1^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \cdots + \xi_{p+q}^2)^2)^{k+m}} \\
&= \frac{1}{(2\pi)^{n/2}((\xi_1^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \cdots + \xi_{p+q}^2)^2)^{k}} \\
&\quad \times \frac{(2\pi)^{n/2}}{(2\pi)^{n/2}((\xi_1^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \cdots + \xi_{p+q}^2)^2)^{m}} \\
&= (2\pi)^{n/2}\mathcal{F}[(-1)^k S_{2k}(x) * R_{2k}(x)]\mathcal{F}[(-1)^m S_{2m}(x) * R_{2m}(x)].
\end{aligned}$$

Since $(-1)^k S_{2(k+m)}(x) * R_{2(k+m)}(x) \in S'$, the space of tempered distribution, and by Theorem 3.1 we obtain that $\mathcal{F}$ is bounded and continuous on S'.

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On the convolutions of the diamond kernel of Marcel Riesz

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Abstract

In this paper, we consider the equation $\Diamond^k u(x) = \delta$ where $\Diamond^k$ is introduced and named as the diamond operator iterated k-times and is defined by $\Diamond^k = ((\sum_{i=1}^{p}(\partial^2/\partial x_i^2))^2 - (\sum_{j=p+1}^{p+q}(\partial^2/\partial x_j^2))^2)^k$, $u(x)$ is a generalized function, $x = (x_1, x_2, \ldots, x_n) \in R^n$ the n-dimensional Euclidean space, $p+q=n$, $k = 0, 1, 2, 3, \ldots$ and δ is the Dirac-delta distribution. Now $u(x)$ is the elementary solution of the operator $\Diamond^k$ and is called the diamond kernel of Marcel Riesz. The main part of this work is studying the convolution of $u(x)$.

Keywords: Diamond kernel; Ultra-hyperbolic kernel; Elliptic kernel; Tempered distribution

1. Introduction

Consider the equation

$$\Diamond^k u(x) = \delta, \tag{1.1}$$

where $\Diamond^k$ is the Diamond operator iterated k-times defined by

$$\Diamond^k = \left(\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \cdots + \frac{\partial^2}{\partial x_p^2}\right)^2 - \left(\frac{\partial^2}{\partial x_{p+1}^2} + \frac{\partial^2}{\partial x_{p+2}^2} + \cdots + \frac{\partial^2}{\partial x_{p+q}^2}\right)^2\right)^k. \tag{1.2}$$

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Kananthai [2, Theorem 3.1] has proved that the convolution solution $u(x) = (-1)^k S_{2k}(x) * R_{2k}(x)$ is the elementary solution of (1.1) where $S_{2k}(x)$ and $R_{2k}(x)$ are defined by (2.2) and (2.4), respectively with $\alpha = 2k$. Now $u(x)$ is called the diamond kernel of Marcel Riesz and defines such a kernel by

$$T_m(x) = (-1)^m S_{2m}(x) * R_{2m}(x), \quad m = 0, 1, 2, \ldots \tag{1.3}$$

In this work we study the existence of $T_m(x) * T_n(x)$ and moreover the inverse T_m^{*-1} of $T_m(x)$ in the convolution algebra $\mathscr{A}'$ is also considered.

2. Preliminaries

Definition 2.1. Let $E(x)$ be a function defined by

$$E(x) = \frac{|x|^{2-n}}{(2-n)\omega_n}, \tag{2.1}$$

where $x = (x_1, x_2, \ldots, x_n) \in R^n$, $|x| = (x_1^2 + x_2^2 + \cdots + x_n^2)^{1/2}$ and $\omega_n = (2\pi^{n/2})/(\Gamma(n/2))$ is a surface area of the unit sphere.

It is well known that $E(x)$ is an elementary solution of the Laplace operator Δ, that $\Delta E(x) = \delta$ where $\Delta = \sum_{i=1}^n \partial^2/\partial x_i^2$ and δ is the Dirac-delta distribution.

Definition 2.2. Let $S_\alpha(x)$ be a function defined by

$$S_\alpha(x) = 2^{-\alpha}\pi^{-n/2}\Gamma\left(\frac{n-\alpha}{2}\right)\frac{|x|^{\alpha-n}}{\Gamma(\alpha/2)}, \tag{2.2}$$

where α is a complex parameter, $|x| = (x_1^2 + x_2^2 + \cdots + x_n^2)^{1/2}$, $x = (x_1, x_2, \ldots, x_n) \in R^n$. $S_\alpha(x)$ is called the elliptic kernel of Marcel Riesz. Now $S_\alpha(x)$ is an ordinary function for $\mathrm{Re}(\alpha) \geqslant n$ and is a distribution of α for $\mathrm{Re}(\alpha) < n$.

From (2.1) and (2.2) we obtain

$$E(x) = -S_2(x) \tag{2.3}$$

and it can be shown that

$$\underbrace{E(x) * E(x) * \cdots * E(x)}_{k\text{-times}} = (-1)^k S_{2k}(x)$$

is the elementary solution of the operator Δ^k iterated k-times that is $\Delta^k(-1)^k S_{2k}(x) = \delta$, see [3].

Definition 2.3. Let $x = (x_1, x_2, \ldots, x_n)$ be a point of R^n and write

$$V = x_1^2 + x_2^2 + \cdots + x_p^2 - x_{p+1}^2 - x_{p+2}^2 - \cdots - x_{p+q}^2, \quad p + q = n.$$

$\Gamma_+ = \{x \in R^n : x_1 > 0 \text{ and } V > 0\}$ designates the interior of the forward cone and denotes $\overline{\Gamma}_+$ by its closure and the following function introduced by Nozaki [4, p. 72] that

$$R_\alpha(x) = \begin{cases} V^{(\alpha-n)/2}/K_n(\alpha) & \text{if } x \in \Gamma_+, \\ 0 & \text{if } x \notin \Gamma_+. \end{cases} \tag{2.4}$$

Here, $R_\alpha(x)$ is called the ultra-hyperbolic kernel of Marcel Riesz and α is a complex parameter and n is the dimension of the space R^n.

The constant $K_n(\alpha)$ is defined by

$$K_n(\alpha) = \frac{\pi^{(n-1)/2}\Gamma((2+\alpha-n)/2)\Gamma((1-\alpha)/2)\Gamma(\alpha)}{\Gamma((2+\alpha-p)/2)\Gamma((p-\alpha)/2)}.$$

Now $R_\alpha(x)$ is an ordinary function if $\mathrm{Re}(\alpha) \geqslant n$ and is a distribution of α if $\mathrm{Re}(\alpha) < n$.

Let supp $R_\alpha(x) \subset \overline{\Gamma}_+$ where supp $R_\alpha(x)$ denotes the support of $R_\alpha(x)$.

Lemma 2.1. *The functions $S_\alpha(n)$ and $R_\alpha(x)$ defined by* (2.2) *and* (2.4) *respectively, for* $\mathrm{Re}(\alpha) < n$ *are Homogeneous distribution of order* $\alpha - n$ *and also a tempered distribution.*

Proof. Since $R_\alpha(x)$ and $S_\alpha(x)$ satisfy the Euler equation, that is

$$(\alpha-n)R_\alpha(x) = \sum_{i=1}^{n} x_i \frac{\partial}{\partial x_i} S_\alpha(x) \quad \text{and} \quad (\alpha-n)S_\alpha(x) = \sum_{i=1}^{n} x_i \frac{\partial}{\partial x_i} R_\alpha(x),$$

we have $R_\alpha(x)$ and $S_\alpha(x)$ are homogeneous distributions of order $\alpha - n$ and Donoghue [1, pp. 154–155] has proved that every homogeneous distribution is a tempered distribution. That completes the proof. □

Lemma 2.2 (The convolution of tempered distributions). *The convolution $S_\alpha(x) * R_\alpha(x)$ exists and is a tempered distribution.*

Proof. Choose supp $R_\alpha(x) = K \subset \overline{\Gamma}_+$ where K is a compact set. Then $R_\alpha(x)$ is a tempered distribution with compact support and by Donoghue [1, pp. 156–159], $S_\alpha(x) * R_\alpha(x)$ exists and is a tempered distribution. □

Lemma 2.3. *Given the equation $\Diamond^k u(x) = \delta$ where $\Diamond^k$ is the operator defined by* (1.2), *$x = (x_1, x_2, \ldots, x_n) \in R^n$, K is a nonnegative integer and δ is the Dirac-delta distribution. Then $u(x) = (-1)^k S_{2k}(x) * R_{2k}(x)$ is the unique elementary solution of the equation where $S_\alpha(x)$ and $R_\alpha(x)$ are defined by* (2.2) *and* (2.4), *respectively with $\alpha = 2k$. Moreover $u(x)$ is a tempered distribution.*

Proof. See [3, Theorem 3.1] and by Lemma 2.2, $u(x) = (-1)^k S_{2k}(x) * R_{2k}(x)$ is a tempered distribution. □

Lemma 2.4 (The convolutions of $R_\alpha(x)$ and $S_\alpha(x)$). *Let $S_\alpha(x)$ and $R_\alpha(x)$ be defined by* (2.2) *and* (2.4) *respectively, then we obtain the following formulas*:
1. $S_\alpha(x) * S_\beta(x) = S_{\alpha+\beta}(x)$, *where α and β are complex parameters.*
2. $R_\alpha(x) * R_\beta(x) = R_{\alpha+\beta}(x)$, *for α and β are both integers and except only the case both α and β are odd integers.*

Proof. Proof of first formula, see [1, p. 158].

Proof of second formula, for the case α and β are both even integers, see [3] and for the case α is odd and β is even or α is even and β is odd, we know from Trione [5] that

$$\square^k R_\alpha(x) = R_{\alpha-2k}(x) \tag{2.5}$$

and

$$\square^k R_{2k} = \delta, \quad k = 0, 1, 2, \ldots \tag{2.6}$$

where $\square^k$ is and ultra-hyperbolic operator iterated k-times ($k = 0, 1, 2, \ldots$) defined by

$$\square^k = \left(\sum_{i=1}^{p} \frac{\partial^2}{\partial x_i^2} - \sum_{j=p+1}^{p+q} \frac{\partial^2}{\partial x_j^2} \right)^k.$$

Now let m be an odd integer, we have

$$\square^k R_m(x) = R_{m-2k}(x)$$

and

$$R_{2k}(x) * \square^k R_m(x) = R_{2k}(x) * R_{m-2k}(x)$$

or

$$(\square^k R_{2k}(x)) * R_m(x) = R_{2k}(x) * R_{m-2k}(x),$$

$$\delta * R_m(x) = R_{2k}(x) * R_{m-2k}(x) \quad \text{by (2.6)},$$

or

$$R_m(x) = R_{2k}(x) * R_{m-2k}(x).$$

Since m is odd, hence $m - 2k$ is odd and $2k$ is a positive even. Put $\alpha = 2k$, $\beta = m - 2k$ we obtain

$$R_\alpha(x) * R_\beta(x) = R_{\alpha+\beta}(x)$$

for α is a nonnegative even and β is odd.

For the case α is a negative even and β is odd, by (2.5) we have

$$\Box^k R_0(x) = R_{-2k}(x) \quad \text{or} \quad \Box^k \delta = R_{-2k}(x)$$

where $R_0(x) = \delta$. Now

$$R_{-2k}(x) * \Box^k R_m(x) = R_{-2k}(x) * R_{m-2k}(x) \quad \text{for } m \text{ is odd,}$$

or

$$(\Box^k \delta) * \Box^k R_m(x) = R_{-2k}(x) * R_{m-2k}(x),$$

$$\delta * \Box^{2k} R_m(x) = R_{-2k}(x) * R_{m-2k}(x),$$

$$R_{m-2(2k)}(x) = R_{-2k}(x) * R_{m-2k}(x).$$

Put $\alpha = -2k$ and $\beta = m - 2k$, now α is a negative even and β is odd. Then we obtain

$$R_\alpha(x) * R_\beta(x) = R_{\alpha+\beta}(x).$$

That completes the proofs. □

3. Main results

Theorem 3.1. *Let $T_m(x)$ the diamond kernel of Marcel Riesz defined by* (1.3), *then T_m is a tempered distribution and can be expressed by*

$$T_m(x) = T_{m-r}(x) * T_r(x),$$

where r is a nonnegative integer and $r < m$. Moreover if we put $\ell = m - r$, $n = r$ we obtain

$$T_\ell(x) * T_n(x) = T_{\ell+n}(x) \quad \textit{for } \ell + n = m.$$

Proof. Since $T_m = (-1)^m S_{2m}(x) * R_{2m}(x)$, $(m = 0, 1, 2, \ldots)$, by Lemma 2.2 T_m is a tempered distribution. Now by Lemma 2.3, $\Diamond^m T_m = \delta$, then $\Diamond^r \Diamond^{m-r} T_m = \delta$ for $m > r$ and by Lemma 2.3 again, we obtain $\Diamond^{m-r} T_m = (-1)^r S_2 r(x) * R_{2r}(x)$. Convolving both sides by $(-1)^{m-r} S_{2(m-r)}(x) * R_{2(m-r)}(x)$, we obtain

$$\begin{aligned}&[(-1)^{m-r} S_{2(m-r)}(x) * R_{2(m-r)}(x)] * \Diamond^{m-r} T_m \\ &\quad = [(-1)^{m-r} S_{2m-2r}(x) * R_{2m-2r}(x)] * [(-1)^r S_{2r}(x) * R_{2r}(x)] \qquad (3.1)\end{aligned}$$

or

$$\begin{aligned}&\Diamond^{m-r}[(-1)^{m-r} S_{2(m-r)}(x) * R_{2(m-r)}(x)] * T_m \\ &\quad = (-1)^m (S_{2m-2r}(x) * S_{2r}(x) * (R_{2m-2r}(x) * R_{2r}(x)),\end{aligned}$$

since $S_{2m}(x)$ and $R_{2m}(x)$ are tempered distributions and are the elements of the space of convolution algebra, $\mathcal{A}'$.

By Lemmas 2.3 and 2.4 we obtain

$$\delta * T_m(x) = (-1)^m S_{2m}(x) * R_{2m}(x),$$
$$T_m(x) = (-1)^m S_{2m}(x) * R_{2m}(x).$$

From (3.1) we have $T_m(x) = T_{m-r}(x) * T_r(x)$, put $\ell = m - r$, $n = r$, it follows that

$$T_\ell(x) * T_n(x) = T_{\ell+n}(x) = T_m(x)$$

as required. □

Theorem 3.2. *Let $T_m(x)$ be defined by* (1.3) *then T_m is an element of the space $\mathcal{A}'$ of convolution algebra and there exist an inverse T_m^{*-1} of T_m such that*

$$T_m(x) * T_m^{*-1} = T_m^{*-1} * T_m(x) = \delta.$$

Proof. Since $T_m(x) = (-1)^m S_{2m}(x) * R_{2m}(x)$ is a tempered distribution by Lemma 2.2. Now the supports of $S_{2m}(x)$ and $R_{2m}(x)$ are compact. Then they are the elements of the space of convolution algebra $\mathcal{A}'$ of distribution. By Zemanian [6, Theorem 6.2.1, p. 151] there exist a unique inverse T_m^{*-1} such that

$$T_m(x) * T_m^{*-1} = T_m^{*-1} * T_m(x) = \delta.$$

That completes the proof. □

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ON THE SPECTRUM OF THE DISTRIBUTIONAL KERNEL RELATED TO THE RESIDUE

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ABSTRACT. We study the spectrum of the distributional kernel $K_{\alpha,\beta}(x)$, where α and β are complex numbers and x is a point in the space $\mathbb{R}^n$ of the n-dimensional Euclidean space. We found that for any nonzero point ξ that belongs to such a spectrum, there exists the residue of the Fourier transform $(-1)^k\widehat{K_{2k,2k}(\xi)}$, where $\alpha=\beta=2k$, k is a nonnegative integer and $\xi\in\mathbb{R}^n$.

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1. Introduction. Gel'fand and Shilov [2, pages 253–256] have studied the generalized function P^λ, where

$$P=\sum_{i=1}^{p}x_i^2-\sum_{j=p+1}^{p+q}x_j^2 \tag{1.1}$$

is a quadratic form, λ is a complex number, and $p+q=n$ is the dimension of $\mathbb{R}^n$. They found that P^λ has two sets of singularities, namely $\lambda=-1,-2,\ldots,-k,\ldots$ and $\lambda=-n/2,-n/2-1,\ldots,-n/2-k,\ldots$, where k is a positive integer. For the singular point $\lambda=-k$, the generalized function P^λ has a simple pole with residue

$$\frac{(-1)^k}{(k-1)!}\delta_1^{(k-1)}(P)\qquad\text{or}\qquad \operatorname{res}_{\lambda=-k}P^\lambda=\frac{(-1)^k}{(k-1)!}\delta_1^{(k-1)}(P) \tag{1.2}$$

for $p+q=n$ is odd with p odd and q even. Also, for the singular point $\lambda=-n/2-k$ they obtained

$$\operatorname{res}_{\lambda=-n/2-k}P^\lambda=\frac{(-1)^{q/2}L^k\delta(x)}{2^{2k}k!\Gamma((n/2)+k)} \tag{1.3}$$

for $p+q=n$ is odd with p odd and q even.

Now, let $K_{\alpha,\beta}(x)$ be the convolution of the functions $R_\alpha^H(u)$ and $R_\beta^\ell(v)$, that is,

$$K_{\alpha,\beta}(x)=R_\alpha^H(u)*R_\beta^\ell(v), \tag{1.4}$$

where $R_\alpha^H(u)$ and $R_\beta^\ell(v)$ are defined by (2.1) and (2.3), respectively. Since $R_\alpha^H(u)$ and $R_\beta^\ell(v)$ are tempered distributions, see [4, pages 30-31], thus $K_{\alpha,\beta}(x)$ is also a tempered distribution and is called the distributional kernel.

In this paper, we use the idea of Gel'fand and Shilov to find the residue of the Fourier transform $(-1)^k\widehat{K_{2k,2k}(\xi)}$, where $K_{2k,2k}$ is defined by (1.4) with $\alpha=\beta=2k$ and k is a nonnegative integer. We found that for any nonzero point ξ that belongs to the spectrum of $(-1)^kK_{2k,2k}(x)$, there exists the residue of the Fourier transform

$(-1)^k\widehat{K_{2k,2k}(\xi)}$. Actually $(-1)^k K_{2k,2k}(x)$ is an elementary solution of the operator $\diamond^k$ iterated k times, that is, $\diamond^k[(-1)^k K_{2k,2k}(x)] = \delta$, where δ is the Dirac-delta distribution.

The operator $\diamond^k$ was first introduced by Kananthai [4] and named as the Diamond operator defined by

$$\diamond^k = \left[\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \cdots + \frac{\partial^2}{\partial x_p^2}\right)^2 - \left(\frac{\partial^2}{\partial x_{p+1}^2} + \frac{\partial^2}{\partial x_{p+2}^2} + \cdots + \frac{\partial^2}{\partial x_{p+q}^2}\right)^2\right]^k, \tag{1.5}$$

where $p+q=n$ is the dimension of $\mathbb{R}^n$.

Moreover, the operator $\diamond^k$ can be expressed as the product of the operators $\square^k$ and $\triangle^k$, that is,

$$\diamond^k = \square^k \triangle^k = \triangle^k \square^k, \tag{1.6}$$

where $\square^k$ is an ultra-hyperbolic operator iterated k times defined by

$$\square^k = \left(\sum_{i=1}^{p} \frac{\partial^2}{\partial x_i^2} - \sum_{j=p+1}^{p+q} \frac{\partial^2}{\partial x_j^2}\right)^k, \tag{1.7}$$

where $p+q=n$. The operator $\triangle^k$ is an elliptic operator or Laplacian iterated k times defined by

$$\triangle^k = \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \cdots + \frac{\partial^2}{\partial x_n^2}\right)^k. \tag{1.8}$$

Trione [7, page 11] has shown that the function $R_{2k}^H(u)$ defined by (2.1) with $\alpha = 2k$ is an elementary solution of the operator $\square^k$. Also, Aguirre Téllez [1, pages 147–148] has proved that the solution $R_{2k}^H(u)$ exists only for odd n with p odd and q even $(p+q=n)$. Moreover, we can show that the function $(-1)^k R_{2k}^{\ell}(v)$ is an elementary solution of the operator $\triangle^k$, where $R_{2k}^{\ell}(v)$ is defined by (2.3) with $\beta = 2k$.

2. Preliminaries

Definition 2.1. Let $x = (x_1, x_2, \ldots, x_n)$ be a point of $\mathbb{R}^n$, and write $u = x_1^2 + x_2^2 + \cdots + x_p^2 - x_{p+1}^2 - \cdots - x_{p+q}^2$, $p+q=n$. Denote by $\Gamma_+ = \{x \in \mathbb{R}^n : x_1 > 0,\ u > 0\}$ the set of an interior of the forward cone, and $\overline{\Gamma_+}$ denotes the closure of Γ_+. For any complex number α, define

$$R_\alpha^H(u) = \begin{cases} \dfrac{u^{(\alpha-n)/2}}{K_n(\alpha)}, & \text{for } x \in \Gamma_+, \\ 0, & \text{for } x \notin \Gamma_+, \end{cases} \tag{2.1}$$

where the constant $K_n(\alpha)$ is given by the formula

$$K_n(\alpha) = \frac{\pi^{(n-1)/2}\Gamma((2+\alpha-n)/2)\Gamma((1-\alpha)/2)\Gamma(\alpha)}{\Gamma((2+\alpha-p)/2)\Gamma((p-\alpha)/2)}. \tag{2.2}$$

The function $R_\alpha^H(u)$ is called the ultra-hyperbolic kernel of Marcel Riesz and was introduced by Nozaki [6, page 72]. The function R_α^H is an ordinary function or classical function if $\mathrm{Re}(\alpha) \geq n$ and is a distribution of α if $\mathrm{Re}(\alpha) < n$. Let $\mathrm{supp} R_\alpha^H(u) \subset \overline{\Gamma_+}$, where $\mathrm{supp} R_\alpha^H(u)$ denotes the support of $R_\alpha^H(u)$.

DEFINITION 2.2. Let $x = (x_1, x_2, \ldots, x_n)$ be a point of $\mathbb{R}^n$, and write $v = x_1^2 + x_2^2 + \cdots + x_n^2$. For any complex number β, define

$$R_\beta^\ell(v) = \frac{2^{-\beta}\pi^{-n/2}\Gamma((n-\beta)/2)v^{(\beta-n)/2}}{\Gamma(\beta/2)}. \tag{2.3}$$

The function $R_\beta^\ell(v)$ is called the elliptic kernel of Marcel Riesz and is an ordinary function for $\mathrm{Re}(\beta) \geq n$ and is a distribution of β for $\mathrm{Re}(\beta) < n$.

DEFINITION 2.3. Let f be a continuous function, then the Fourier transform of f, denoted by $\mathfrak{I}f$ or $\hat{f}(\xi)$, is defined by

$$\mathfrak{I}f = \hat{f}(\xi) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-i(\xi,x)} f(x)dx, \tag{2.4}$$

where $x = (x_1, x_2, \ldots, x_n) \in \mathbb{R}^n$, $\xi = (\xi_1, \xi_2, \ldots, \xi_n) \in \mathbb{R}^n$, and $(\xi, x) = \xi_1 x_1 + \xi_2 x_2 + \cdots + \xi_n x_n$. From (2.4), the inverse Fourier transform of $\hat{f}(\xi)$ is defined by

$$f(x) = \mathfrak{I}^{-1}\hat{f}(\xi) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{i(\xi,x)} \hat{f}(\xi)dx. \tag{2.5}$$

If f is a distribution with compact support, by [8, Theorem 7.4.3, page 187] (2.5) can be written as

$$\mathfrak{I}f = \hat{f}(\xi) = \frac{1}{(2\pi)^{n/2}} \langle f(x), e^{-i(\xi,x)} \rangle. \tag{2.6}$$

LEMMA 2.4. *Given the equation*

$$\diamond^k u(x) = \delta, \tag{2.7}$$

where $\diamond^k$ is the operator defined by (1.5), and δ is the Dirac-delta distribution, $u(x)$ is an unknown, k is a nonnegative integer and $x \in \mathbb{R}^n$, where n is odd with p odd, q even $(n = p + q)$. Then $u(x) = (-1)^k K_{2k,2k}(x)$ is an elementary solution of the operator $\diamond^k$. Here $K_{2k,2k}(x) = R_{2k}^H(u) * R_{2k}^\ell(v)$ from (1.4) with $\alpha = \beta = 2k$.

PROOF. See [4, page 33]. □

In this paper, we study the spectrum of $(-1)^k K_{2k,2k}(x)$, relate to the residue of the Fourier transform $(-1)^k \widehat{K_{2k,2k}(\xi)}$.

LEMMA 2.5. *The Fourier transform*

$$\begin{aligned} \widehat{K_{\alpha,\beta}(\xi)} &= (2\pi)^{n/2} \mathfrak{I}R_\alpha^H(u) \mathfrak{I}R_\beta^\ell(v) \\ &= \frac{(i)^q 2^{\alpha+\beta}\pi^n}{(2\pi)^{n/2} K_n(\alpha) H_n(\beta)} \cdot \frac{\Gamma(\alpha/2)\Gamma(\beta/2)}{\Gamma((n-\alpha)/2)\Gamma((n-\beta)/2)} \\ &\quad \times \left(\sqrt{\sum_{i=1}^{p} \xi_i^2 - \sum_{j=p+1}^{p+q} \xi_j^2} \right)^{-\alpha} \left(\sqrt{\sum_{i=1}^{n} \xi_i^2} \right)^{-\beta}, \quad i = \sqrt{-1}. \end{aligned} \tag{2.8}$$

In particular, if $\alpha = \beta = 2k$, k is a nonnegative integer,

$$(-1)^k \widehat{K_{2k,2k}(\xi)} = \frac{1}{(2\pi)^{n/2}} \frac{1}{((\xi_1^2+\xi_2^2+\cdots+\xi_p^2)^2-(\xi_{p+1}^2+\xi_{p+2}^2+\cdots+\xi_{p+q}^2)^2)^k}, \quad (2.9)$$

where $R_\alpha^H(u)$ and $R_\beta^\ell(v)$ are defined by (2.1) and (2.3), respectively.

PROOF. See [2, page 194] and [5, pages 156–157]. □

DEFINITION 2.6. The spectrum of the distributional kernel $K_{\alpha,\beta}(x)$ is the support of the Fourier transform $\widehat{K_{\alpha,\beta}(\xi)}$ or the spectrum of $K_{\alpha,\beta}(x) = \operatorname{supp}\widehat{K_{\alpha,\beta}(\xi)}$. Now, from Lemma 2.5 we obtain

$$\operatorname{supp}\widehat{K_{\alpha,\beta}(\xi)} = (\operatorname{supp}\Im R_\alpha^H(u)) \cap (\operatorname{supp}\Im R_\beta^\ell(v)). \quad (2.10)$$

In particular, from (2.9) the spectrum of

$$(-1)^k K_{2k,2k}(x) = \operatorname{supp}\left[\frac{1}{(2\pi)^{n/2}((\sum_{i=1}^p \xi_i^2)^2-(\sum_{j=p+1}^{p+q}\xi_j^2)^2)^k}\right]. \quad (2.11)$$

LEMMA 2.7. *Let $P(x_1,x_2,\ldots,x_n)$ be a quadratic form of positive definite, and is defined by*

$$P = P(x_1,x_2,\ldots,x_n) = \left(\sum_{i=1}^p x_i^2\right)^2 - \left(\sum_{j=p+1}^{p+q} x_j^2\right)^2, \quad (2.12)$$

then for any testing function $\varphi(x) \in D$, the space of infinitely differentiable function with compact support,

$$\langle \delta^{(k)}(P), \varphi\rangle = \int_0^\infty \left[\left(\frac{\partial}{4s^3\partial s}\right)^k \left(s^{q-4}\frac{\psi(r,s)}{4}\right)\right]_{s=r} r^{p-1}\,dr, \quad (2.13)$$

$$\langle \delta^{(k)}(P), \varphi\rangle = (-1)^k \int_0^\infty \left[\left(\frac{\partial}{4r^3\partial r}\right)^k \left(r^{p-4}\frac{\psi(r,s)}{4}\right)\right]_{r=s} s^{q-1}\,ds, \quad (2.14)$$

where $r^2 = x_1^2+x_2^2+\cdots+x_p^2$, $s^2 = x_{p+1}^2+x_{p+2}^2+\cdots+x_{p+q}^2$, and

$$\psi(r,s) = \int \varphi\, d\Omega^p d\Omega^q, \quad (2.15)$$

where $d\Omega^p$ and $d\Omega^q$ are the elements of surface area on the unit sphere in $\mathbb{R}^p$ and $\mathbb{R}^q$, respectively. Both integrals (2.13) and (2.14) converge if $k < (1/4)(p+q-4)$ for any $\varphi(x) \in D$. If $k \geq (1/4)(p+q-4)$, these integrals must be understood in the sense of their regularization and (2.13) defined as $\langle \delta_1^{(k)}(p), \varphi\rangle$ and (2.14) defined as $\langle \delta_2^{(k)}(p), \varphi\rangle$. Moreover, if we put $u = r^2$, $v = s^2$, thus (2.13) and (2.14) become

$$\langle \delta^{(k)}(p), \varphi\rangle = \frac{1}{16}\int_0^\infty \left[\frac{\partial^k}{\partial v^k}(v^{(q-4)/4}\psi_1(u,v))\right]_{v=u} u^{(1/4)(p-4)}\,du, \quad (2.16)$$

$$\langle \delta^{(k)}(p), \varphi\rangle = \frac{(-1)^k}{16}\int_0^\infty \left[\frac{\partial^k}{\partial u^k}(u^{(p-4)/4}\psi_1(u,v))\right]_{u=v} v^{(1/4)(q-4)}\,dv, \quad (2.17)$$

where $\psi_1(u,v) = \psi(r,s)$.

PROOF. See [2, pages 247-251]. □

LEMMA 2.8. *Let $G_b = \{\xi \in \mathbb{R}^n : |\xi_1| \le b_1, |\xi_2| \le b_2, \ldots, |\xi_n| \le b_n\}$ be a parallelepiped in $\mathbb{R}^n$ and b_i $(1 \le i \le n)$ is a real constant and the inverse Fourier transform of $\widehat{K_{\alpha,\beta}(\xi)}$ is defined by*

$$K_{\alpha,\beta}(x) = \mathfrak{I}^{-1}\widehat{K_{\alpha,\beta}(\xi)} = \frac{1}{(2\pi)^{n/2}} \int_{G_b} e^{i(\xi,x)} \widehat{K_{\alpha,\beta}(\xi)}\, d\xi, \tag{2.18}$$

where $K_{\alpha,\beta}$ is defined by (1.4) and $x, \xi \in \mathbb{R}^n$, then $K_{\alpha,\beta}(x)$ can be extended to the entire function $K_{\alpha,\beta}(z)$ and be analytic for all $z = (z_1, z_2, \ldots, z_n) \in \mathbb{C}^n$, where $\mathbb{C}^n$ is the n-tuple space of complex number and

$$|K_{\alpha,\beta}(z)| \le C \exp(b\,|\operatorname{Im}(z)|), \tag{2.19}$$

where $\exp(b|\operatorname{Im}(z)|) = \exp[b_1|\operatorname{Im}(z_1)| + b_2|\operatorname{Im}(z_2)| + \cdots + b_n|\operatorname{Im}(z_n)|]$ and $C = (1/(2\pi)^{n/2}) \int_{G_b} |\widehat{K_{\alpha,\beta}(\xi)}|\, d\xi$ is a constant. Moreover, $K_{\alpha,\beta}(x)$ has a spectrum contained in G_b.

PROOF. Since the integral of (2.18) converges for all $\xi \in G_b$, thus $K_{\alpha,\beta}(x)$ can be extended to the entire function $K_{\alpha,\beta}(z)$ and be analytic for all $z \in C^n$. Thus (2.18) can be written as

$$K_{\alpha,\beta}(z) = \frac{1}{(2\pi)^{n/2}} \int_{G_b} e^{i(\xi,z)} \widehat{K_{\alpha,\beta}(\xi)}\, d\xi. \tag{2.20}$$

Now,

$$\begin{aligned} |K_{\alpha,\beta}(z)| &\le \frac{1}{(2\pi)^{n/2}} \int_{G_b} |\widehat{K_{\alpha,\beta}(\xi)}|\, |\exp(i\xi_1 z_1 + i\xi_2 z_2 + \cdots + i\xi_n z_n)|\, d\xi \\ &= \frac{1}{(2\pi)^{n/2}} \int_{G_b} |\widehat{K_{\alpha,\beta}(\xi)}|\, |\exp(i\xi_1\sigma_1 + i\xi_2\sigma_2 + \cdots + i\xi_n\sigma_n \\ &\qquad - \xi_1\mu_1 - \xi_2\mu_2 - \cdots - \xi_n\mu_n)|\, d\xi, \end{aligned} \tag{2.21}$$

where

$$z_j = \sigma + i\mu_j \quad (j = 1, 2, \ldots, n), \tag{2.22}$$

thus

$$|K_{\alpha,\beta}(z)| \le \frac{1}{(2\pi)^{n/2}} \int_{G_b} |\widehat{K_{\alpha,\beta}(\xi)}|\, d\xi \exp(b_1|\mu_1| + b_2|\mu_2| + \cdots + b_n|\mu_n|) \tag{2.23}$$

for $|\xi_j| \le b_j$, or $|K_{\alpha,\beta}(z)| \le C\exp(b_1|\operatorname{Im}(z_1)| + b_2|\operatorname{Im}(z_2)| + \cdots + b_n|\operatorname{Im}(z_n)|)$, or $|K_{\alpha,\beta}(z)| \le C\exp(b|\operatorname{Im}(z)|)$, where $C = (1/(2\pi)^{n/2}) \int_{G_b} |\widehat{K_{\alpha,\beta}(\xi)}|\, d\xi$ is a constant. □

We must show that the support of $\widehat{K_{\alpha,\beta}(\xi)}$ is contained in G_b. Since $K_{\alpha,\beta}(z)$ is an analytic function that satisfies the inequality (2.19) and is called an entire function of order of growth ≤ 1 and of type $\le b$, then by Paley-Wiener-Schartz theorem, see [3, page 162], $\widehat{K_{\alpha,\beta}(\xi)}$ has a support contained in G_b, that is the spectrum of $K_{\alpha,\beta}(x)$ is contained in G_b.

In particular, for $\alpha = \beta = 2k$, the spectrum of $(-1)^k K_{2k,2k}(x)$ is also contained in G_b, that is $\operatorname{supp}[(-1)^k \widehat{K_{2k,2k}(\xi)}] \subset G_b$, where $(-1)^k K_{2k,2k}(x)$ is an elementary solution of the Diamond operator $\diamond^k$ by Lemma 2.4, and the Fourier transform $(-1)^k \widehat{K_{2k,2k}(\xi)}$ given by (2.9) can be defined as follows.

Definition 2.9. The Fourier transform

$$(-1)^k \widehat{K_{2k,2k}(\xi)} = \begin{cases} \dfrac{1}{(2\pi)^{n/2}\left[\left(\sum_{i=1}^{p} \xi_i^2\right)^2 - \left(\sum_{j=p+1}^{p+q} \xi_j^2\right)^2\right]^k}, & \text{for } \xi \in G_b, \\ 0, & \text{for } \xi \in CG_b, \end{cases} \tag{2.24}$$

where $\xi = (\xi_1, \xi_2, \ldots, \xi_n) \in \mathbb{R}^n$ and CG_b is the complement of G_b.

3. Main results

Theorem 3.1. *For any nonzero point $\xi \in M$ where M is a spectrum of $(-1)^k K_{2k,2k}(x)$, and $(-1)^k K_{2k,2k}(x)$ is an elementary solution of the operator $\diamond^k$ by Lemma 2.4. Then there exists the residue of the Fourier transform $(-1)^k \widehat{K_{2k,2k}(\xi)}$ at the singular point $\lambda = -k$ and such a residue is*

$$\frac{(-1)^{k-1}}{(2\pi)^{n/2}(k-1)!}\delta_1^{(k-1)(p)} \quad \text{or} \quad \operatorname{res}_{\lambda=-k}(-1)^k \widehat{K_{2k,2k}(\xi)} = \frac{(-1)^{k-1}}{(2\pi)^{n/2}(k-1)!}\delta^{(k-1)(p)}, \tag{3.1}$$

where

$$P = (\xi_1^2 + \xi_2^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \xi_{p+2}^2 + \cdots + \xi_{p+q}^2), \tag{3.2}$$

$p + q = n$ and $\delta_1^{(k-1)}(P)$ is defined by (2.16) with $\delta^{(k-1)}(P) = \delta_1^{(k-1)}(P)$ and n is odd with p odd, q even.

Proof. We define the generalized function P^λ, where P is given by (3.2) and λ is a complex number, by

$$\langle P^\lambda, \varphi \rangle = \int_{P>0} P^\lambda(\xi)\varphi(\xi)d\xi, \tag{3.3}$$

where $\xi = (\xi_1, \xi_2, \ldots, \xi_n)$ and $d\xi = d\xi_1 d\xi_2 \cdots d\xi_n$ and $\varphi(\xi) \in D$, the space of continuous infinitely differentiable function with compact support. Now,

$$\langle P^\lambda, \varphi \rangle = \int_{P>0} [(\xi_1^2 + \xi_2^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \xi_{p+2}^2 + \cdots + \xi_{p+q}^2)]^\lambda \varphi(\xi)d\xi. \tag{3.4}$$

We transform to bipolar coordinates defined by

$$\begin{gathered} \xi_1 = rw_1,\ \xi_2 = rw_2,\ \ldots,\ \xi_p = rw_p, \\ \xi_{p+1} = sw_{p+1},\ \xi_{p+2} = sw_{p+2},\ \ldots,\ \xi_{p+q} = sw_{p+q}, \quad p+q = n, \end{gathered} \tag{3.5}$$

where $\sum_{i=1}^{p} w_i^2 = 1$ and $\sum_{j=p+1}^{p+q} w_j^2 = 1$. Thus

$$r = \sqrt{\sum_{i=1}^{p} \xi_i^2}, \qquad s = \sqrt{\sum_{j=p+1}^{p+q} \xi_j^2}. \tag{3.6}$$

We have $\langle P^\lambda, \varphi\rangle = \int [r^4 - s^4]^\lambda \varphi(\xi) d\xi$. Since the volume $d\xi = r^{p-1}s^{q-1}\,dr\,ds\,d\Omega_p\,d\Omega_q$ where $d\Omega_p$ and $d\Omega_q$ are the elements of surface area on the unit sphere in $\mathbb{R}^p$ and $\mathbb{R}^q$, respectively. Thus

$$\begin{aligned}\langle P^\lambda, \varphi\rangle &= \int_{p>0} (r^4 - s^4)^\lambda \varphi r^{p-1}s^{q-1}\,dr\,ds\,d\Omega^p\,d\Omega^q \\ &= \int_0^\infty \int_0^r (r^4 - s^4)^\lambda \psi(r,s) r^{p-1}s^{q-1}\,ds\,dr,\end{aligned} \tag{3.7}$$

where $\psi(r,s) = \int \varphi\, d\Omega_p\, d\Omega_q$.

Since $\varphi(\xi)$ is in D, then $\psi(r,s)$ is an infinitely differentiable function of r^4 and s^4 with bounded support. We now make the change of variable $u = r^4$, $v = s^4$, and writing $\psi(r,s) = \psi_1(u,v)$. Thus we obtain

$$\langle P^\lambda, \varphi\rangle = \frac{1}{16}\int_{u=0}^\infty \int_{v=0}^u (u-v)^\lambda \psi_1(u,v) u^{(p-4)/4} v^{(q-4)/4}\,dv\,du. \tag{3.8}$$

Write $v = ut$. We obtain

$$\langle P^\lambda, \varphi\rangle = \frac{1}{16}\int_0^\infty u^{\lambda+(1/4)(p+q)-1}\,du \int_0^1 (1-t)^\lambda t^{(q-4)/4}\psi_1(u,ut)\,dt. \tag{3.9}$$

Let the function

$$\Phi(\lambda,u) = \frac{1}{16}\int_0^1 (1-t)^\lambda t^{(q-4)/4}\psi_1(u,ut)\,dt. \tag{3.10}$$

Thus $\Phi(\lambda,u)$ has singularity at $\lambda = -k$ where it has simple poles. By Gel'fand and Shilov [2, page 254, equation (12)] we obtain the residue of $\Phi(\lambda,u)$ at $\lambda = -k$, that is,

$$\operatorname{res}_{\lambda=-k}\Phi(\lambda,u) = \frac{1}{16}\frac{(-1)^{k-1}}{(k-1)!}\left[\frac{\partial^{k-1}}{\partial t^{k-1}}\{t^{(q-4)/4}\psi_1(u,ut)\}\right]_{t=1}. \tag{3.11}$$

Thus, $\operatorname{res}_{\lambda=-k}\Phi(\lambda,u)$ is a functional concentrated on the surface $P = 0$ ($t = 1$, $u = v$, $p = u - v = 0$). On the other hand, from (3.9) and (3.10) we have

$$\langle P^\lambda, \varphi\rangle = \int_0^\infty u^{\lambda+(1/4)(p+q)-1}\Phi(\lambda,u)\,du. \tag{3.12}$$

Thus $\langle P^\lambda, \varphi\rangle$ in (3.12) has singularities at $\lambda = -n/4, -n/4-1, \ldots, -n/4-k$. At these points,

$$\operatorname{res}_{\lambda=-n/4-k}\langle P^\lambda, \varphi\rangle = \frac{1}{k!}\left[\frac{\partial^k}{\partial u^k}\Phi\left(-\frac{n}{4}-k, u\right)\right]_{u=0}. \tag{3.13}$$

Thus the residue of $\langle P^\lambda, \varphi\rangle$ at $\lambda = (-1/2)n - k$ is a functional concentrated on the vertex of the surface P. Now consider the case when the singular point $\lambda = -k$. Write (3.10) in the neighborhood of $\lambda = -k$ in the form $\Phi(\lambda,u) = \Phi_0(u)/(\lambda+k) + \Phi_1(\lambda,u)$ where $\Phi_0(u) = \operatorname{res}_{\lambda=-k}\Phi(\lambda,u)$ and $\Phi_1(\lambda,u)$ is regular at $\lambda = -k$. Substitute $\Phi(\lambda,u)$ into (3.12) we obtain

$$\langle P^\lambda, \varphi\rangle = \frac{1}{\lambda+k}\int_0^\infty u^{\lambda+(1/4)(p+q)-1}\Phi_0(u)\,du + \int_0^\infty u^{\lambda+(1/4)(p+q)-1}\Phi_1(\lambda,u)\,du. \tag{3.14}$$

Thus $\operatorname{res}_{\lambda=-k}\langle P^\lambda,\varphi\rangle = \int_0^\infty u^{-k+(1/4)(p+q)-1}\Phi_0(u)\,du$. By substituting $\Phi_0(u)$ and (3.11), we obtain

$$\operatorname{res}_{\lambda=-k}\langle P^\lambda,\varphi\rangle = \frac{(-1)^k}{16(k-1)!}\int_0^\infty \left[\frac{\partial^{k-1}}{\partial t^{k-1}}\{t^{1(q-4)/4}\psi_1(u,ut)\}\right]_{t=1} u^{-k+(1/4)(p+q)-1}\,du \tag{3.15}$$

since, we put $v = ut$. Thus $\partial^{k-1}/\partial t^{k-1} = u^{k-1}(\partial^{k-1}/\partial v^{k-1})$, by substituting $\partial^{k-1}/\partial t^{k-1}$ we obtain

$$\operatorname{res}_{\lambda=-k}\langle P^\lambda,\varphi\rangle = \frac{(-1)^k}{16(k-1)!}\int_0^\infty \left[\frac{\partial^{k-1}}{\partial t^{k-1}}\{v^{1(q-4)/4}\psi_1(u,v)\}\right]_{u=v} u^{(1/4)p-1}\,du. \tag{3.16}$$

Now, by (2.16)

$$\operatorname{res}_{\lambda=-k}\langle P^\lambda,\varphi\rangle = \frac{(-1)^{k-1}}{(k-1)!}\delta_1^{(k-1)}(P). \tag{3.17}$$

Since, by Definition 2.9 we have

$$(-1)^k\widehat{K_{2k,2k}(\xi)} = \frac{1}{(2\pi)^{n/2}}P^\lambda \quad \text{for } \lambda = -k, \tag{3.18}$$

and $\xi \in G_b$. Let M be a spectrum of $(-1)^k K_{2k,2k}(x)$ and $M \subset G_b$ by Lemma 2.8. Thus for any nonzero $\xi \in M$ we can find the residue of $(-1)^k\widehat{K_{2k,2k}(\xi)}$, that is,

$$\begin{aligned}\operatorname{res}_{\lambda=-k}\langle(-1)^k\widehat{K_{2k,2k}(\xi)},\varphi(\xi)\rangle &= \frac{1}{(2\pi)^{n/2}}\operatorname{res}_{\lambda=-k}\langle P^\lambda,\varphi\rangle \\ &= \frac{(-1)^{k-1}}{(2\pi)^{n/2}(k-1)!}\langle\delta_1^{(k-1)}(P),\varphi\rangle\end{aligned} \tag{3.19}$$

or $\operatorname{res}_{\lambda=-k}(-1)^k\widehat{K_{2k,2k}(\xi)} = ((-1)^{k-1}/(2(\pi)^{n/2}(k-1)!))\delta_1^{(k-1)}(P)$ for $\xi \in M$ and $\xi \neq 0$.

Now consider the case $\xi = 0$. We have from (3.13) that, the residue of $\langle P^\lambda,\varphi\rangle$ occurs at the point $\lambda = (-1/2)n-k$ that is $\operatorname{res}_{\lambda=-(1/2)n-k}\langle P^\lambda,\varphi\rangle$ is a functional concentrated on the vertex of surface P. Since $u = 0$ and $v = ut$, then $u = v = 0$, that implies

$$\sqrt{\xi_1^2+\xi_2^2+\cdots+\xi_p^2} = \sqrt{\xi_{p+1}^2+\xi_{p+2}^2+\cdots+\xi_{p+q}^2} = 0. \tag{3.20}$$

It follows that $\xi_1 = \xi_2 = \cdots = \xi_{p+q} = 0$, $p+q = n$. Thus, the residue of $\langle P^\lambda,\varphi\rangle$ is concentrated on the point $\xi = 0$.

Since, from Definition 2.9, $(1/(2\pi)^{n/2})P^\lambda = (-1)^k\widehat{K_{2k,2k}(\xi)}$ if $\lambda = -k$. Thus we only consider the residue of $(-1)^k\widehat{K_{2k,2k}(\xi)}$ at $\lambda = -k$. From (3.12), we consider the residue of $\langle P^\lambda,\varphi\rangle$ only at $\lambda = -k$. That implies $(1/4)(p+q)-1 = 0$ or $n = 4$ $(p+q = n)$. Since $n = 4$ is an even dimension which contradicts Lemma 2.4, the existence of the elementary solution $(-1)^k K_{2k,2k}(x)$ that exists for odd n. Thus cases (3.12) and (3.13) do not occur. This implies that the case $\xi = 0$ does not happen. It follows that

$$\operatorname{res}_{\lambda=-k}(-1)^k\widehat{K_{2k,2k}(\xi)} = \frac{(-1)^{k-1}}{(2\pi)^{n/2}(k-1)!}\delta_1^{(k-1)}(P) \tag{3.21}$$

for nonzero point $\xi \in M$ concentrated on the surface $P = 0$, where M is a spectrum of $(-1)^k K_{2k,2k}(x)$. □

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On the Diamond Operator related to the Wave Equation

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Abstract

In this paper, we study the solution of the equation $\Diamond^k u(x) = f(x)$ where $\Diamond^k$ is the Diamond operator iterated k times and is defined by

$$\Diamond^k = \left(\left(\sum_{i=1}^{p} \frac{\partial^2}{\partial x_i^2} \right)^2 - \left(\sum_{j=p+1}^{p+q} \frac{\partial^2}{\partial x_j^2} \right)^2 \right)^k$$

where $p+q=n$ is the dimension of the n-dimensional Euclidean space $R^n, x = (x_1, x_2, ..., x_n) \in R^n$, k is a nonnegative integer, $u(x)$ is an unknown and f is a generalized function.

It is found that the solution $u(x)$ depends on the conditions of p and q and moreover such a solution is related to the solution of the Laplace equation and the wave equation.

1 Introduction

The operator $\Diamond^k$ has been first introduced by A. Kananthai [3] and is named as the Diamond operater iterated k times and is defined by

$$\begin{aligned} \Diamond^k \;=\; & \left(\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \cdots + \frac{\partial^2}{\partial x_p^2} \right)^2 - \right. \\ & \left. \left(\frac{\partial^2}{\partial x_{p+1}^2} + \frac{\partial^2}{\partial x_{p+2}^2} + \cdots + \frac{\partial^2}{\partial x_{p+q}^2} \right)^2 \right)^k \end{aligned} \tag{1.1}$$

where $p+q=n$ is the dimension of the space $R^n, x = (x_1, x_2, ..., x_n) \in R^n$ and k is a nonnegative integer.

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Actually the operator $\Diamond^k$ is an extension of the ultrahyperbolic operator and the Laplacian. So the operator $\Diamond^k$ can be expressed as the product of the operator $\Box$ and $\triangle$, that is $\Diamond^k = \Box^k \triangle^k = \triangle^k \Box^k$ where

$$\Box^k = \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \cdots + \frac{\partial^2}{\partial_p^2} - \frac{\partial^2}{\partial x_{p+1}^2} - \frac{\partial^2}{\partial x_{p+2}^2} - \cdots - \frac{\partial^2}{\partial x_{p+q}^2} \right)^k \tag{1.2}$$

is the ultrahyperbolic operator iterated k-time with $p+q=n$, and

$$\triangle^k = \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \cdots + \frac{\partial^2}{\partial x_n^2} \right)^k \tag{1.3}$$

is the Laplacian iterated k-times.

A. Kananthai ([3], Theorem 3.1 p33) has shown that the convolution $(-1)^k R_{2k}^e(x) * R_{2k}^H(x)$ is an elementory solution of the operator $\Diamond^k$, that is

$$\Diamond^k \left((-1)^k R_{2k}^e(x) * R_{2k}^H(x) \right) = \delta \tag{1.4}$$

where δ is the Dirac-delta distribution and the functions R_{2k}^e and R_{2k}^H are defined by (2.5) and (2.1) respectively with $\alpha = 2k, k$ is nonnegative integer.

In this paper, we study the solution of the equation

$$\Diamond^k u(x) = f(x) \tag{1.5}$$

This equation is the geheralization of the ultrahyperbolic equation and it can be applied to the wave equation and potential that has been shown in the last part of this paper.

Let $K_{\alpha,\beta}(x)$ be a distributional family and is defined by

$$K_{\alpha,\beta}(x) = R_\alpha^e * R_\beta^H \tag{1.6}$$

where R_α^e is called the elliptic Kernel defined by (2.5) and R_β^H is called the ultra-hyperbolic Kernel defined by (2.1) and α, β are the complex parameters.

The family $K_{\alpha,\beta}(x)$ is well-defined and is a tempered distribution, since $R_\alpha^e * R_\beta^H$ is a tempered, see ([1], Lemma 2.2) and R_β^H has a compact support.

In this paper, we can show that

$$u(x) = (-1)^k R_{2k}^e(x) * \left(R_{2(k-1)}^H(v) \right)^{(m)} + (-1)^k K_{2k,2k}(x) * f(x)$$

is a solution of (1.5) where m $= \frac{n-4}{2}, n \geq 4$ and n is even number and $k_{2k,2k}(x)$ is defined by (1.6) with $\alpha = \beta = 2k$. Moreover, we can show that the solution u(x) relates to the solution of Laplace operator $\triangle^{2k}$ defined by (1.3)and also the wave operator defined by (1.2) with $k=1$ and $p=1$.

2 Preliminaries

Definition 2.1 Let $x = (x_1, x_2, ..., x_n)$ be a point of the n-dimensional Euclidean space R^n.

Denote by $v = x_1^2 + x_2^2 + \cdots + x_p^2 - x_{p+1}^2 - x_{p+2}^2 - \cdots - x_{p+q}^2, p + q = n$ the nondegenerated quadratic form. By Γ_+ we designate the interior of the forward cone.

$\Gamma_+ = \{x \in R^n : x_1 > 0 and v > 0\}$, and by $\overline{\Gamma}_+$ designate its closure. For any complex number α, define

$$R_\alpha^H(v) = \begin{cases} \frac{v^{(\alpha-n)/2}}{K_n(\alpha)} & \text{for } x \in \Gamma_+ \\ 0 & \text{for } x \notin \Gamma_+ \end{cases} \tag{2.1}$$

where $K_n(\alpha)$ is given by the formula

$$K_n(\alpha) = \frac{\pi^{(n-1)/2}\Gamma\left(\frac{2+\alpha-n}{2}\right)\Gamma\left(\frac{1-\alpha}{2}\right)\Gamma(\alpha)}{\Gamma\left(\frac{2+\alpha-p}{2}\right)\Gamma\left(\frac{p-\alpha}{2}\right)}. \tag{2.2}$$

The function $R_\alpha^H(x)$ was introduced by Nozaki ([4], p.72).

It is well known that $R_\alpha^H(x)$ is an ordinary function if $Re(\alpha) \geq n$ and it is a distribution of α if $Re(\alpha) < n$. Let $\text{supp}R_\alpha^H(x)$ denote the support of $R_\alpha^H(x)$. Suppose that $\text{supp}R_\alpha^H(x) \subset \overline{\Gamma}_+$.

From S.E Trione ([5], p11), $R_{2k}^H(v)$ is an elementary solution of the operator $\Box^k$ that is

$$\Box^k R_{2k}^H(v) = \delta \tag{2.3}$$

where $\Box^k$ is defined by (1.2).

By putting $p = 1$ in (2.1) and (2.2) and remembering the Legendre's duplication of $\Gamma(z)$.

$\Gamma(2z) = 2^{2z-1}\pi^{-1/2}\Gamma(z)\Gamma\left(z + \frac{1}{2}\right)$ then the formula (2.1) reduces to

$$M_\alpha(v) = \begin{cases} \frac{v^{(\alpha-n)/2}}{H_n(\alpha)} & \text{if } x \in \Gamma_+ \\ 0 & \text{if } x \notin \Gamma_+ \end{cases} \tag{2.4}$$

Here $v = x_1^2 - x_2^2 - \cdots - x_n^2$ and $H_n(\alpha) = \pi^{(n-2)/2}2^{\alpha-1}\Gamma\left(\frac{\alpha-n+2}{2}\right)\Gamma\left(\frac{\alpha}{2}\right)$.

$M_\alpha(v)$ is, precisely, the hyperbolic kernel of Marcel Riesz.

Definition 2.2 Let $x = (x_1, x_2, ..., x_n)$ be a point of R^n and the function $R_\alpha^e(x)$ be defined by

$$R_\alpha^e(x) = \frac{|x|^{\alpha-n}}{W_n(\alpha)} \tag{2.5}$$

where $W_n(\alpha) = \frac{\pi^{n/2}2^\alpha\Gamma\left(\frac{\alpha}{2}\right)}{\Gamma\left(\frac{n-\alpha}{2}\right)}$, α is a complex parameter and $|x| = (x_1^2 + x + 2^2 + \cdots + x_n^2)^{1/2}$.

It can be shown that $R_{-2k}^e(x) = (-1)^k\triangle^k\delta(x)$ where $\triangle^k$ is defined by (1.3). It follows that $R_0^e(x) = \delta$, see ([2], p118).

Moreover, we obtain $(-1)^k R^e_{2k}(x)$ is an elementary solution of the operator $\triangle^k$, that is

$$\triangle^k \left((-1)^k R^e_{2k}(x)\right) = \delta \tag{2.6}$$

see ([3] , Lemma 2.4 p31).

Lemma 2.1 Given P is a hyper-surface then

$$P\delta^{(k)}(P) + k\delta^{(k-1)}(P) = 0$$

where $\delta^{(k)}$ is the Dirac-delta distribution with k derivatives.
Proof. See ([1], P233).

Lemma 2.2 Given the equation

$$\triangle^k u(x) = 0 \tag{2.7}$$

where $\triangle^k$ is defined by (1.3) and $x = (x_1, x_2, ..., x_n) \in R^n$ then $u(x) = (-1)^{(k-1)} \left(R^e_{2(k-1)}(x)\right)^{(m)}$ is a solution of (2.7) where m is a nonnegative integer with $m = \frac{n-4}{2}, n \geq 4$ and n is even and $\left(R^e_{2(k-1)}(x)\right)^{(m)}$ is a function defined by (2.5) with m derivatives with $\alpha = 2(k-1)$
Proof. We first show that the generalized function $u(x) = \delta^{(m)}(r^2)$ where $r^2 = |x|^2 = x_1^2 + x_2^2 + \cdots + x_n^2$ is a solution of

$$\triangle u(x) = 0 \tag{2.8}$$

where $\triangle = \sum_{i=1}^n \frac{\partial^2}{\partial x_i^2}$ is a Laplace operator.Now

$$\begin{aligned} \frac{\partial}{\partial x_i}\delta^{(m)}(r^2) &= 2x_i\delta^{(m+1)}(r^2) \\ \frac{\partial^2}{\partial x_i^2}\delta^{(m)}(r^2) &= 2\delta^{(m+1)}(r^2) + 4x_i^2\delta^{(m+2)}(r^2). \end{aligned}$$

Thus

$$\begin{aligned} \triangle\delta^{(m)}(r^2) &= \sum_{i=1}^n \frac{\partial^2}{\partial x_i^2}\delta^{(m)}(r^2) \\ &= 2n\delta^{(m+1)}(r^2) + 4r^2\delta^{(m+2)}(r^2) \\ &= 2n\delta^{(m+1)}(r^2) - 4(m+2)\delta^{(m+1)}(r^2) \end{aligned}$$

by Lemma 2.1 with $P = r^2$.We have

$$\begin{aligned} \triangle\delta^{(m)}(r^2) &= [2n - 4(m+2)]\delta^{(m+1)}(r^2) \\ &= 0 \quad \text{if } 2n - 4(m+2) = 0 \end{aligned}$$

or $m = \frac{n-4}{2}, n \geq 4$ and n is even. Thus $\delta^{(m)}(r^2)$ is a solution of (2.8) with $m = \frac{n-4}{2}, n \geq 4$ and n is even. Now $\triangle^k u(x) = \triangle(\triangle^{k-1}u(x)) = 0$ then from the above proof $\triangle^{k-1}u(x) = \delta^{(m)}(r^2)$ with $m = \frac{n-4}{2}, n \geq 4$ and n is even.

Convolving both sides of the above equation by the function $(-1)^{k-1}R^e_{2(k-1)}(x)$, we obtain

$$\begin{aligned}(-1)^{k-1}R^e_{2(k-1)}(x) * \triangle^{k-1}u(x) &= (-1)^{k-1}R^e_{2(k-1)}(x) * \delta^{(m)}(r^2)\\ \text{or } \triangle^{k-1}\left((-1)^{k-1}R^e_{2(k-1)}(x)\right) * u(x) &= (-1)^{k-1}R^e_{2(k-1)}(x) * \delta^{(m)}(r^2)\end{aligned}$$

$$\text{or} \qquad \delta * u(x) = u(x) = (-1)^{k-1}R^e_{2(k-1)}(x) * \delta^{(m)}(r^2) \quad \text{by (2.6)}$$

Now from (2.1)

$$\begin{aligned}R^e_{2(k-1)}(x) &= \frac{|x|^{2(k-1)-n}}{W_n(\alpha)}\\ &= \frac{\left(|x|^2\right)^{\frac{2(k-1)-n}{2}}}{W_n(\alpha)} = \frac{\left(r^2\right)^{\frac{2(k-1)-n}{2}}}{W_n(\alpha)}\end{aligned}$$

where $r = |x| = (x_1^2 + x_2^2 + \cdots + x_n^2)^{1/2}$. Hence

$$\begin{aligned}R^e_{2(k-1)}(x) * \delta^{(m)}(r^2) &= \frac{\left(r^2\right)^{\frac{2(k-1)-n}{2}}}{W_n(\alpha)} * \delta^{(m)}(r^2)\\ &= \left[\frac{\left(r^2\right)^{\frac{2(k-1)-n}{2}}}{W_n(\alpha)}\right]^{(m)} = \left[R^e_{2(k-1)}(x)\right]^{(m)}.\end{aligned}$$

It follows that $u(x) = (-1)^{k-1}\left[R^e_{2(k-1)}(x)\right]^{(m)}$ is a solution of (2.7) with $m = \frac{n-4}{2}, n \geq 4$ and n is even dimension of R^n.

Lemma 2.3 Given the equation

$$\Box^k u(x) = 0 \tag{2.9}$$

where $\Box^k$ is defined by (1.2) and $x = (x_1, x_2, ..., x_n) \in R^n$ then $u(x) = \left[R^H_{2(k-1)}(v)\right]^{(m)}$ is a solution of (2.9) with $m = \frac{n-4}{n}, n \geq 4$ and n is even dimension and v is defined by Definition 2.1. The function $\left[R^H_{2(k-1)}(v)\right]^{(m)}$ is defined by (2.1) with m-derivatives and $\alpha = 2(k-1)$.

Proof At first we show that the generalized function $\delta^{(m)}(r^2 - s^2)$ where $r^2 = x_1^2 + x_2^2 + \cdots + x_p^2$ and $s^2 = x_{p+1}^2 + x_{p+2}^2 + \cdots + x_{p+q}^2, p + q = n$, is a solution of the equation

$$\Box u(x) = 0 \tag{2.10}$$

where $\Box$ is defined by (1.2) with $k = 1$ and $x = (x_1, x_2, ..., x_n) \in R^n$. Now

$$\begin{aligned}
\frac{\partial}{\partial x_i}\delta^{(m)}(r^2-s^2) &= 2x_i\delta^{(m+1)}(r^2-s^2)\\
\frac{\partial^2}{\partial x_i^2}\delta^{(m)}(r^2-s^2) &= 2\delta^{(m+1)}(r^2-s^2)+4x_i^2\delta^{(m+2)}(r^2-s^2)\\
\sum_{i=1}^{p}\frac{\partial^2}{\partial x_i^2}\delta^{(m)}(r^2-s^2) &= 2p\delta^{(m+1)}(r^2-s^2)+4r^2\delta^{(m+2)}(r^2-s^2)\\
&= 2p\delta^{(m+1)}(r^2-s^2)\\
&\quad +4(r^2-s^2)\delta^{(m+2)}(r^2-s^2)\\
&\quad +4s^2\delta^{(m+2)}(r^2-s^2)\\
&= 2p\delta^{(m+1)}(r^2-s^2)\\
&\quad -4(m+2)\delta^{(m+1)}(r^2-s^2)\\
&\quad +4s^2\delta^{(m+2)}(r^2-s^2)\\
&= [2p-4(m+2)]\delta^{(m+1)}(r^2-s^2)\\
&\quad +4s^2\delta^{(m+2)}(r^2-s^2)
\end{aligned}$$

by Lemma 2.1 with $P=r^2-s^2$.
Similarly,

$$\begin{aligned}
\sum_{j=p+1}^{p+q}\frac{\partial^2}{\partial x_j^2}\delta^{(m)}(r^2-s^2) &= [-2q+4(m+2)]\delta^{(m+1)}(r^2-s^2)\\
&\quad +4r^2\delta^{(m+2)}(r^2-s^2).
\end{aligned}$$

Thus

$$\begin{aligned}
\Box\delta^{(m)}(r^2-s^2) &= \sum_{i=1}^{p}\frac{\partial^2}{\partial x_i^2}\delta^{(m)}(r^2-s^2)-\sum_{j=p+1}^{p+q}\frac{\partial^2}{\partial x_j^2}\delta^{(m)}(r^2-s^2)\\
&= [2(p+q)-8(m+2)]\delta^{(m+1)}(r^2-s^2)\\
&\quad -4(r^2-s^2)\delta^{(m+2)}(r^2-s^2)\\
&= [2n-8(m+2)]\delta^{(m+1)}(r^2-s^2)\\
&\quad +4(m+2)\delta^{(m+1)}(r^2-s^2)\quad \text{by Lemma 2.1}\\
&= [2n-4(m+2)]\delta^{(m+1)}(r^2-s^2).
\end{aligned}$$

If $2n-4(m+2)=0$, we have $\Box\delta^{(m)}(r^2-s^2)=0$. That is $u(x)=\delta^{(m)}(r^2-s^2)$ is a solution of (2.10) with $m=\frac{n-4}{2}, n\geq 4$ and n is even dimension. Now $\Box^k u(x)=\Box\left(\Box^{k-1}u(x)\right)=0$.

From (2.10) we have $\Box^{k-1}u(x)=\delta^{(m)}(r^2-s^2)$ with $m=\frac{n-4}{2}, n\geq 4$ and n is even dimension.

Convolving the above equation by $R^H_{2(k-1)}(v)$, we obtain

$$\begin{aligned}
R^H_{2(k-1)}(v)*\Box^{k-1}u(x) &= R^H_{2(k-1)}(v)*\delta^{(m)}(r^2-s^2)\\
\Box^{k-1}\left[R^H_{2(k-1)}(v)\right]*u(x) &= \left[R^H_{2(k-1)}(v)\right]^{(m)} \text{ where } v=r^2-s^2\\
\delta*u(x)=u(x) &= \left[R^H_{2(k-1)}(v)\right]^{(m)}
\end{aligned}$$

by (2.3) and $v=r^2-s^2$ is defined by Definition 2.1.

Thus $u(x)=\left[R^H_{2(k-1)}(v)\right]^{(m)}$ is a solution of (2.9) with $m=\frac{n-4}{2}, n\geq 4$ and n is even dimension.

Lemma 2.4 Given the equation

$$\Diamond^k u(x) = 0 \tag{2.11}$$

where $\Diamond^k$ is the Diamond operator iterated k-times defined by (1.1) and $u(x)$ is an unknown generalized function.Then

$$u(x) = (-1)^k R^e_{2k}(x) * \left(R^H_{2(k-1)}(v)\right)^{(m)} \tag{2.12}$$

is a solution of (2.11), $\left(R^H_{2(k-1)}(v)\right)^{(m)}$ is a function with m-derivatives defined by (2.1) and v is defined by definition 2.1.

Proof Now $\Diamond^k u(x) = \Box^k \triangle^k u(x) = 0$. By Lemma 2.3 ,$\triangle^k u(x) = \left(R^H_{2(k-1)}(v)\right)^{(m)}$.

Convolving both sides by $(-1)^k R^e_{2k}(x)$, we have

$$(-1)^k R^e_{2k}(x) * \triangle^k u(x) = (-1)^k R^e_{2k}(x) * \left(R^H_{2(k-1)}(v)\right)^{(m)}.$$

By (2.6), $\triangle^k \left((-1)^k R^e_{2k}(x)\right) * u(x) = \delta * u(x) = (-1)^k R^e_{2k}(x) * \left(R^H_{2(k-1)}(v)\right)^{(m)}$. It follows that

$$u(x) = (-1)^k R^e_{2k}(x) * \left(R^H_{2(k-1)}(v)\right)^{(m)}. \tag{2.13}$$

3 Main results

Theorem Given The equation

$$\Diamond^k u(x) = f(x) \tag{3.1}$$

where $\Diamond^k$ is the Diamond operator iterated k-times defined by (1.1), $f(x)$ is a generalized function, $u(x)$ is an unknown generalized function and $x = (x_1, x_2, ...x_n) \in R^n$-the n-dimensional Euclidean space and n is even, then (3.1) has the general solution

$$u(x) = (-1)^k R^e_{2k}(x) * \left(R^H_{2(k-1)}(v)\right)^{(m)} + (-1)^k K_{2k,2k}(x) * f(x) \tag{3.2}$$

where $\left(R^H_{2(k-1)}(v)\right)^{(m)}$ is a function with m-derivatives defined by (2.1) and $K_{2k,2k}(x)$ is defined by (1.6) with $\alpha = \beta = 2k$.

Proof Convolving (3.1) both sides by $(-1)^k K_{2k,2k}(x)$, we obtain

$$(-1)^k K_{2k,2k}(x) * \Diamond^k u(x) = (-1)^k K_{2k,2k}(x) * f(x).$$

By (1.4) $\Diamond^k \left((-1)^k K_{2k,2k}(x)\right) * u(x) = \delta * u(x) = (-1)^k K_{2k,2k}(x) * f(x)$. We obtain $u(x) = (-1)^k K_{2k}(x) * f(x)$. Since, for a Homogeneous equation $\Diamond^k u(x) = 0$ we have a solution $u(x) = (-1)^k R^e_{2k}(x) * \left(R^H_{2(k-1)}(v)\right)^{(m)}$.

Thus the general solution of (3.1) is

$$u(x) = (-1)^k R^e_{2k}(x) * \left(R^H_{2(k-1)}(v)\right)^{(m)} + (-1)^k K_{2k,2k}(x) * f(x).$$

In particular, if $q = 0$ the equation (3.1) becomes the Laplace equation $\triangle^{2k} u(x) = f(x)$ where $x = (x_1, x_2, x_3, ..., x_p) \in R^p$ and p is even. Using the formulae $\Gamma(2z) = 2^{2z-1}\pi^{-1/2}\Gamma(z)\Gamma(z + \frac{1}{2})$ and $\Gamma(\frac{1}{2} + z)\Gamma(\frac{1}{2} - z) = \pi sec(\pi z)$. Then for $\alpha = 2k$ the function of (2.1) becomes $(-1)^k R^e_{2k}(x)$ where $R^e_{2k}(x)$ is defined by (2.5) and $x = (x_1, x_2, ..., x_p) \in R^p$. Thus by (1.6)

$$\begin{aligned}(-1)^k K_{2k,2k}(x) &= (-1)^k R^e_{2k}(x) * (-1)^k R^e_{2k}(x) \\ &= R^e_{4k}(x) \text{ see ([2], p156-159)}\end{aligned}$$

where $x = (x_1, x_2, ..., x_p) \in R^p$ and p is even.

Now, from (2.12) for $q = 0$ we have

$$\begin{aligned}u(x) &= (-1)^k R^e_{2k}(x) * (-1)^{k-1} \left(R^e_{2(k-1)}(x)\right)^{(m)} \\ &= (-1)^{2k-1} \left(R^e_{4k-2}(x)\right)^{(m)} \quad \text{for } x = (x_1, x_2, ..., x_p) \in R^p.\end{aligned}$$

Thus the equation (3.2) becomes

$$u(x) = (-1)^{2k-1} \left(R^e_{4k-2}(x)\right)^{(m)} + R^e_{4k}(x) * f(x) \tag{3.3}$$

for $x = (x_1, x_2, ..., x_p) \in R^p$ and p is even.
It follows that (3.3) is the general solution of the Laplace equation $\triangle^{2k} u(x) = f(x)$ where $\triangle^{2k}$ is the Laplace operator iterated $2k$-times defined by (1.3) for $x = (x_1, x_2, ..., x_n) \in R^n$ and n is even.

Now consider the case for the Wave Equation. Given the equation

$$\Box^k V(x) = f(x) \tag{3.4}$$

where $f(x)$ is a generalized function,$\Box^k$ is defined by (1.2) and $V(x)$ is an unknown function. By ([5],p11) we obtain $V(x) = R^H_{2k}(v) * f(x)$ is a solution of (3.4) where $R^H_{2k}(v)$ is defined by (2.1).

Now, from (3.1) we have $u(x) = (-1)^k K_{2k,2k}(x) * f(x)$ is a solution where $K_{2k,2k}(x)$ is defined by (1.6) with $\alpha = \beta = 2k$ or

$$u(x) = \left[(-1)^k R^e_{2k}(x) * R^e_{2k}(v)\right] * f(x) \tag{3.5}$$

Convolving both sides of (3.5) by $(-1)^k R^e_{-2k}(x)$, we obtain

$$\begin{aligned}(-1)^k R^e_{-2k}(x) * u(x) &= \left((-1)^{2k} R^e_{-2k}(x) * R^e_{2k}(x)\right) * R^H_{2k}(v) * f(x) \\ &= \left(R^e_0(x) * R^H_{2k}(v)\right) * f(x) \\ &= \left(\delta * R^H_{2k}(v)\right) * f(x) \\ &= R^H_{2k}(v) * f(x) \quad \text{see ([2],p156-159)}\end{aligned}$$

Thus it follows that

$$V(x) = (-1)^k R^e_{-2k}(x) * u(x) \tag{3.6}$$

In particular, for $k = 1$, we obtain $V(x) = R^H_2(v) * f(x)$ is a solution of the equation

$$\Box V(x) = f(x). \tag{3.7}$$

If we put $p = 1$ and $x_1 = t$(time),then $\Box = \frac{\partial^2}{\partial t^2} - \sum_{i=2}^{n} \frac{\partial^2}{\partial x_i^2}$ is the wave operator. Thus (3.7) becomes wave equation,

$$\left(\frac{\partial^2}{\partial t^2} - \sum_{i=2}^{n} \frac{\partial^2}{\partial x_i^2} \right) V(x) = f(x) \tag{3.8}$$

Thus $V(x) = M_2(v) * f(x)$ is a solution of (3.8) and the general solution of (3.8) is $V(x) = \delta^{(m)}(v) + M_2(v) * f(x)$ where $\delta^{(m)}(v)$ is a solution for $f(x) = 0$ $v = t^2 - x_2^2 - x_3^2 - \cdots - x_n^2$ and $M_2(v)$ is defined by (2.4) with $v = t^2 - x_2^2 - x_3^2 - \cdots - x_n^2$.

Now in (3.1),put $k = 1$ and by (3.2) we obtain

$$\begin{aligned} u(x) &= (-1)R^e_2(x) * \left(R^H_0(v)\right)^{(m)} + (-1)K_{2,2}(x) * f(x) \\ &= (-1)R^e_2(x) * \delta^{(m)}(v) + (-1)K_{2,2}(x) * f(x) \end{aligned} \tag{3.9}$$

is a solution of the equation $\Diamond u(x) = f(x)$ and by (3.6) with $k = 1, V(x) = (-1)R^e_{-2}(x) * u(x)$ is a solution of (3.7) where $u(x)$ is defined by (3.9). Thus

$$\begin{aligned} V(x) &= (-1)R^e_{-2}(x) * ((-1)R^e_2(x) * \delta^{(m)}(v)) \\ &\quad +(-1)R^e_{-2}(x) * ((-1)K_{2,2}(x) * f(x)) \\ &= \left(R^e_{-2}(x) * R^e_2(x)\right) * \delta^{(m)}(v) \\ &\quad +(R^e_{-2}(x) * R^e_2(x)) * R^H_2(x) * f(x) \\ &= R^e_0(x) * \delta^{(m)}(v) + R^e_0(x) * (R^H_2(x) * f(x)) \\ &= \delta^{(m)}(v) \div R^H_2(x) * f(x) \qquad (R^e_0(x) = \delta) \end{aligned} \tag{3.10}$$

where $v = x_1^2 + x_2^2 + \cdots + x_p^2 - x_{p+1}^2 - x_{p+2}^2 - \cdots - x_{p+q}^2$, $p + q = n$.
Now, if we put $p = 1$ and $x_1 = t$, then (3.10) becomes $V(x) = \delta^{(m)}(v) + M_2(v) * f(x)$ since $R^H_2(x)$ becomes $M_2(v)$ for $v = t^2 - x_2^2 - x_3^2 - \cdots - x_n^2$ where $M_2(v)$ is defined by (2.4) with $\alpha = 2$. Thus $V(x) = \delta^{(m)}(v) + M_2(v) * f(x)$ is the general solution of the wave equation (3.8) and $\delta^{(m)}(v)$ is a solution of

$$\left(\frac{\partial^2}{\partial t^2} - \sum_{i=2}^{n} \frac{\partial^2}{\partial x_i^2} \right) V(x) = 0 \tag{3.11}$$

Now $v = t^2 - x_2^2 - x_3^2 - \cdots - x_n^2$, let $r^2 = x_2^2 + x_3^2 + \cdots + x_n^2$. Thus by ([1],p234-236) we obtain $V(x,t) = \delta^{(m)}(t^2 - r^2)$ is the solution of (3.11) with the initial conditions $V(x,0) = 0$ and $\frac{\partial V(x,0)}{\partial t} = (-1)^m 2\pi^{m+1}\delta(x)$ at $t = 0$ and $x = (x_2, x_3, ..., x_n) \in R^{n-1}$.

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