

# รายงานฉบับสมบูรณ์

สัญญาเลขที่ RTA/07/2538

โครงการ A Proposal for Upgrading the Forum for Theoretical  
Science (FTS) to be a Centre of Theoretical Science

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ชื่อหัวหน้าโครงการ ศาสตราจารย์ ดร. วิรุฬห์ สายคณิต  
สถานที่ติดต่อ ฟอรัมวิทยาศาสตร์ทฤษฎี  
ห้อง 206 ตึกฟิสิกส์ 1  
คณะวิทยาศาสตร์  
จุฬาลงกรณ์มหาวิทยาลัย  
กรุงเทพ 10330  
โทร. (02) 218 5111 และ 218 5113  
โทรสาร (02)255 2775

โครงการ : 1 ตุลาคม 2538 ถึง 30 กันยายน 2541

ผู้ให้ทุนสนับสนุนโครงการ : สำนักงานกองทุนสนับสนุนการวิจัย (สกว.)

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ชื่อหัวหน้าโครงการ

ศาสตราจารย์ ดร. วิรุฬห์ สายคณิต

• สถานที่ติดต่อ

ฟอรัมวิทยาศาสตร์ทฤษฎี

ห้อง 206 ตึกฟิสิกส์ 1

คณะวิทยาศาสตร์

จุฬาลงกรณ์มหาวิทยาลัย

กรุงเทพ 10330

โทร. (02) 218 5111 และ 218 5113

โทรสาร (02) 255 2775

ระยะเวลาของโครงการ

1 ตุลาคม 2538 ถึง 30 กันยายน 2541

ผู้ให้ทุนสนับสนุนโครงการ

สำนักงานกองทุนสนับสนุนการวิจัย(สกว.)

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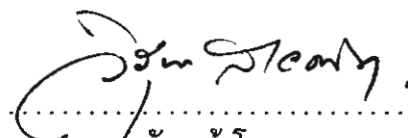
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ชื่อหัวหน้าโครงการ ศาสตราจารย์ ดร. วิรุพท์ สายคณิต  
สถานที่ติดต่อ ฟอรัมวิทยาศาสตร์ทฤษฎี  
ห้อง 206 ตึกฟิสิกส์ 1  
คณะวิทยาศาสตร์  
จุฬาลงกรณ์มหาวิทยาลัย  
กรุงเทพ 10330  
โทร. (02) 218 5111 และ 218 5113  
โทรสาร (02) 255 2775

ระยะเวลาของโครงการ 1 ตุลาคม 2538 ถึง 30 กันยายน 2541

ผู้ให้ทุนสนับสนุนโครงการ สำนักงานกองทุนสนับสนุนการวิจัย(สกว.)

ลงนาม

  
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หัวหน้าโครงการ

วันที่ 19 ตุลาคม 2541

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## บทคัดย่อ

ฟอรัมวิทยาศาสตร์ทฤษฎี (FTS) ก่อตั้งขึ้นในปี พ.ศ. 2529 โดยมีวัตถุประสงค์เพื่อยกระดับมาตรฐานการค้นคว้าวิจัยทางด้านฟิสิกส์ทฤษฎีและคณิตศาสตร์ ซึ่งจุฬาลงกรณ์มหาวิทยาลัยได้ตระหนักถึงความสำคัญและได้ให้การสนับสนุนทางการเงินโดยทันที

เป้าหมายหมายของ FTS เริ่มเป็นจริงมากขึ้นเรื่อย ๆ ดังจะเห็นได้จากผลงานวิจัยในแต่ละปีที่ผ่านมามีคุณภาพเพิ่มมากขึ้นอย่างเห็นได้ชัด โดยเฉพาะในสามปีที่ผ่านมาภายใต้การสนับสนุนทางการเงินจากสำนักงานกองทุนสนับสนุนการวิจัย(สกว.) ที่เพิ่มมากขึ้นถือได้ว่าเป็นการเพิ่มศักยภาพและการพัฒนา เพื่อให้ FTS เป็นศูนย์กลางความเป็นเลิศเทียบเท่ามาตรฐานสากลได้สัมฤทธิ์ผลเพิ่มขึ้นเป็นอย่างมาก

การเพิ่มการสนับสนุนทางการเงินแก่ FTS นับเป็นการตัดสินใจที่ดีเยี่ยม ทำให้เกิดการพัฒนทางด้านฟิสิกส์และคณิตศาสตร์ขึ้นเป็นอย่างมากในประเทศไทย และการพัฒนาครั้งนี้ นับเป็นก้าวกระโดดที่สำคัญสู่ความเป็นสากล ดังจะเห็นได้จาก

1. ผลงานที่ได้รับการตีพิมพ์ลงในวารสารระดับสากลอันดับหนึ่งทางด้านฟิสิกส์ 6 ผลงาน
2. มีความร่วมมือกับนักฟิสิกส์ที่มีชื่อเสียงหลายท่าน จากสถาบันวิทยาศาสตร์ที่ได้รับการเชื่อถือในต่างประเทศ โดยการเชิญนักฟิสิกส์เหล่านั้นมาพำนักในประเทศไทยเป็นเวลานาน และนอกจากนี้ FTS ยังสร้างความร่วมมือระหว่างนักวิทยาศาสตร์ภายในประเทศอีกด้วย
3. จัดให้มีการประชุมทางวิชาการนานาชาติขึ้นในประเทศไทย เพื่อให้ให้นักวิทยาศาสตร์ภายในประเทศมีโอกาสได้รับความรู้เพิ่มเติมจากนักวิทยาศาสตร์ต่างประเทศ ทั้งโดยการบรรยายเป็นทางการและจากการพูดคุยกัน
4. สร้างนักศึกษาระดับบัณฑิตศึกษาที่มีคุณภาพ โดยผลงานของนักศึกษาเหล่านี้บางส่วนได้รับการตีพิมพ์ในวารสารระดับสากลชั้นนำทางด้านฟิสิกส์
5. ประสานความร่วมมือทางด้านคณิตศาสตร์ระหว่าง จุฬาลงกรณ์มหาวิทยาลัย มหาวิทยาลัยเชียงใหม่ และมหาวิทยาลัยเทคโนโลยีสุรนารี
6. สนับสนุนให้นักวิทยาศาสตร์ในประเทศเดินทางไปประชุมที่ต่างประเทศในสาขาวิชาที่ตนเองมีความชำนาญ

7. จัดหาหนังสือ วารสาร ที่มีคุณภาพ และอุปกรณ์สื่อสารทางไกลเพื่อให้นักวิจัยในประเทศได้รับความก้าวหน้า รวมทั้งผลงานใหม่ ๆ ทั้งในด้านฟิสิกส์และคณิตศาสตร์ได้อย่างรวดเร็ว
8. จัดการประชุมประจำปีเพื่อนำเสนอความสำเร็จของ FTS ต่อ สกว. โดยการประชุมเมื่อวันที่ 17 กันยายน 2541 เป็นการประชุมครั้งที่ 3 และเป็นครั้งสุดท้ายสำหรับเงินทุนที่ได้รับในระยะเวลา 3 ปีที่ผ่านมา

ความสำเร็จที่เกิดขึ้นคงจะลดน้อยลงกว่านี้มากหากไม่ได้รับการสนับสนุนที่ดีเยี่ยมจาก สกว. นอกจากความสำเร็จที่กล่าวมานี้การสนับสนุนจากสกว. ยังได้สร้างสรรค์ให้เกิดบรรยากาศของการวิจัยที่เป็นอิสระตามแรงบันดาลใจของนักวิทยาศาสตร์ทั้งหลายที่เกิดขึ้น ท่านที่กำลังอ่านรายงานฉบับนี้ย่อมจะมองเห็นได้ไม่ยากว่า ความสำเร็จที่ FTS ได้รับนั้นเกิดขึ้นได้อย่างไร และเป็นประโยชน์ต่อประเทศของเราอย่างไร

พวกเรากำลังมองไปข้างหน้าถึงความสำเร็จที่จะได้รับ โดยการสนับสนุนทางการเงินจาก สกว. อีก 3 ปี พวกเราหวังเป็นอย่างยิ่งว่าจะสามารถประสบความสำเร็จมากกว่าที่เคยประสบจากสามปีที่ผ่านมาโดยการสนับสนุนอย่างดียิ่งของ สกว.

## Abstract

Forum for Theoretical Science (FTS) was founded in 1986 with the purpose of raising the low standard of research in theoretical sciences and mathematics. Chulalongkorn University realized the importance of this goal and immediately gave financial support to FTS.

The goal of FTS was progressively being realized, each year the quality of research was improving significantly. Three years ago the Thailand Research Fund (TRF) recognizing the achievements of FTS gave significant financial support to FTS in order to accelerate its growth towards becoming a center of excellence with respect to international standards.

This was a wise decision because with the additional funding FTS was able to do much more to develop physics and mathematics in Thailand. We have taken a very big step towards international standards as is shown by the following:

- 1) six publications in international physics journals of the first order
- 2) collaboration with many outstanding physicists from highly respected scientific institutions abroad and also establishing cooperation between scientists in Thailand. This was done by inviting them to come to Thailand for long stays.
- 3) holding international conferences in Thailand so that local scientists can learn from internationally established foreign scientists both by formal lectures and informal talks.
- 4) graduating graduate students whose theses are of such good quality that some of them were published in the best physics journals.
- 5) co-ordinating mathematics activity between Chulalongkorn University, Chiang Mai University and the Suranaree University of Technology.
- 6) supporting local scientists to go to conferences abroad that are directly related to their fields of expertise.
- 7) obtaining the best books and telecommunications equipment so that local researchers can get the latest results in both physics and mathematics immediately.
- 8) holding yearly conferences to demonstrate to the TRF what our accomplishments were. The 17 September 1998 conference was the third and final conference for the three year period of our last grant.

These excellent achievements would be greatly diminished without the generous support of the TRF. We now have created an exciting atmosphere where ideas are

flowing freely and inspiring all scientists in Thailand. Anyone reading the details of the report can easily see the details of what FTS has achieved. It is a valuable asset and resource of our country.

We look forward to what we can attain with the second three year grant from the TRF. We are very optimistic that we can accomplish even more than we did with the first three year grant.

โครงการ A Proposal for Upgrading the Forum for Theoretical Science (FTS) to be a  
Centre of Theoretical Science

**Final Report**  
on the Accomplishments of  
Forum for Theoretical Science (FTS)  
Faculty of Science, Chulalongkorn University

**Introduction**

FTS receives a three-year grant from the Thailand Research Fund (TRF) to support its research and academic activities. This report summarizes the hitherto achievements of FTS so that the TRF can evaluate the progress that FTS has made under its support.

FTS is very happy to say that during the last three years the results of our efforts have been outstanding, far beyond what we expected when we wrote our proposal to the TRF three years ago.

**Summary of our Accomplishments**

In order to describe our accomplishments we shall discuss them in the same order that we listed the expectations in our proposal three years ago (see Appendix 1). It is recommended that the readers have a copy of the proposal written three years ago and turn to the section describing expectations.

**1) Facility Improvement**

*The first and foremost area that we listed in our proposal concerned communications and library facilities. In order to keep up to date with the latest developments in science and mathematics, one needs good computer facilities e.g. the Internet. In order to know the latest results, one needs a good library consisting of journals and textbooks. The journals are needed so that one knows what has already been done and what remains unknown. However the textbooks are of great importance because one cannot enter a new field of study by reading only papers in journals as they are written for experts. To enter a new field one needs textbooks. Textbooks are indispensable for all, especially students.*

### ***1.1 Computers***

We start with computers. FTS has eight pentium PCs to allow many graduate students to calculate. Many problems in contemporary physics cannot be solved analytically and physicists must resort to approximation using computations on a computer. Also graduate students must search the Internet to see if others are working in his area or related areas so he does not duplicate what is already known.

We have developed a 266 MHz Pentium to run UNIX and to be a Web-and-mail server. Information of FTS and related physics will be installed on this server. Internet users can then fetch information from the URL <http://fts.sc.chula.ac.th> or <http://161.200.117.20> when our web-page is done. We plan to obtain a faster computer to run UNIX and share all the computer facilities within the group.

### ***1.2 Journals***

Concerning our journals we are happy to say that we now subscribe to all copies of the Physical Review B. In the past we only had the Physical Review for the first fifteen days of the month. Now we also subscribe to Physical Review B15 giving us all issues of this journal which is the most important physics journal.

We do not feel the need to subscribe to other physics journals because some of them are already in the physics department library or the faculty of science library. Specialized journals are in the physics department library and general physics journals are in the faculty of science's library.

### ***1.3 Books***

Finally, our library has the most complete collection of books on the Feynman Path Integral and the Wiener Integral. These books are for all our members but they are indispensable for our Ph.D. students and visiting physicists. Foreign visitors in this field, have no need of leaving FTS's room for references.

Prof. Virulh Sa-yakanit, the director of FTS, has been working for 30 years to improve the library. During this period at least 300 new physics books have been obtained. We must acknowledge the International Centre for Theoretical Physics (ICTP) for many of these books given from their book donation program.

## **2) Seminars**

The second area that we listed in our proposal concerned holding a regular weekly general seminar where our staff at FTS can communicate with others their latest ideas in order to get feedback and new directions in their research. We envisioned that visiting foreign staff would also participate both in giving lectures and in listening to our local staff.

We are happy to say that the weekly seminar has been very regular. It was mostly attended by graduate students, both Master's and Ph.D. students. The students read papers of deep relevance to physics in the future. Prof. Virulh Sa-yakanit with his vast experience and stature in the physics community chose the papers because he knew what was important.

As a result of the weekly seminar the quality of the FTS students improved immensely. In fact, one student published his M.Sc. thesis in *Physical Review*, the most prestigious physics journal.

Of course, when we had visiting physicists they also gave lectures. In addition, whenever physicists passed through Bangkok we invited them to give us a talk at our seminar.

Overall, the program was a big success.

## **3) Annual Meetings**

The third area that we listed in our proposal concerned holding regular annual meeting here in Thailand in both physics and mathematics in order to bring outstanding physicists and mathematicians from all over the world here so that all Thai physicists and mathematicians can benefit from their lectures and informal conversations with them.

### **3.1 Mathematics**

Our mathematics director Dr. Sidney S. Mitchell conceived of and organized a "Workshop on Algebraic Analysis" that was held at Suranaree University of technology from 20 January to 2 February 1997. Seven of Japan's outstanding analysts spoke on different areas of analysis. They are:

- 3.1.1 Prof. H. Araki of the Science University of Tokyo spoke on Operator Algebras
- 3.1.2 Prof. T. Oshima of the University of Tokyo spoke on homogeneous spaces and representations of Lie Group

- 3.1.3 Prof. M. Morimoto of Sophia University spoke on Hyperfunctions
- 3.1.4 Prof. M. Hayashi of Hokkaido University spoke on Commutative Banach Algebras
- 3.1.5 Prof. S. Watanabe of Kyoto University spoke on Wiener Measures
- 3.1.6 Prof. H. Omori of the Science University of Tokyo spoke on Noncommutative Differential Geometry
- 3.1.7 Dr. A. Nakabayashi of Kyushu University spoke on the XXZ model
- 3.1.8 Wayne Lawton of the National University of Singapore who spoke on Wavelet theory
- 3.1.9 I. Kvasov of SUT who spoke on splines
- 3.1.10 Moshkin of SUT who spoke on the Finite Difference Method and
- 3.1.11 V. Meleshko of SUT who spoke on partial differential equations.

We expect to publish the papers that the speakers presented in the near future.

### ***3.2 Physics***

Concerning physics meetings, FTS was deeply involved in helping Thailand obtain its first synchrotron radiation machine and as a result its main meetings in Thailand centered around the theme of Synchrotron Radiation.

- 3.2.1 The first big meeting held in Thailand took place at Chulalongkorn University from 3-7 January 1996 and was entitled "Applications of Synchrotron Radiation". Twenty lectures were given, all by physicists from developed countries.
- 3.2.2 The second big meeting sponsored by FTS was a major undertaking. It was a four-week meeting held at Suranaree University in February 1997 and it was entitled "School on Applications of Synchrotron Radiation". Its purpose was to train local scientists on how to use the synchrotron radiation machine.

The other two meetings were of duration one day but they were nevertheless very well attended and the lectures were very good.

- 3.2.3 The first meeting was held at Chulalongkorn University on 11 September 1996 and was entitled "First Meeting on Theoretical Physics with Special Lectures on Bose-Einstein Condensation and

Fractional Quantum Hall Effect". All the lecturers were employees of Thai universities except for Professors Wolfgang Weller and Vladimir S. Yarunin, two internationally, recognized physicists.

- 3.2.4 The second meeting was the "Second Meeting on Theoretical Physics Topics in Disordered Systems". It was held on 25 September 1997 at Chulalongkorn University. Five long lectures were presented, Two by Prof. Virulh Sa-yakanit, one by Dr. Gabriella Slavcheva of the Bulgarian Academy of Sciences, one by Dr. Wichit Sritrakool and one by a graduate student at FTS, Mr. Kobchai Tayanasanti.
- 3.2.5 Finally, as promised, FTS held its regular annual meeting for 1998 at Chulalongkorn University on Thursday 17 September 1998. Its title was "Third Meeting in Theoretical Physics : Feynman's Path Integrals and Theoretical Physics". The title is very good because it covered a broad range of theoretical physics as one can see by looking at the program. Another good point about the meeting was the inclusion of two outstanding Thai mathematicians who lectured on Analysis, a very important field of mathematics which has many applications in physics.

Prof. Virulh Sa-yakanit was the first speaker and he gave a history and an overview of the Feynman Path Integral to the audience. It was a perfect beginning because the Feynman Path Integral has been applied to almost every field of theoretical physics. It is worth mentioning that most of the audience consisted of Thai graduate students in physics and this talk contained knowledge that they will need in their future careers in physics. After gaining this basic background, the other physics lecturers went into more specific areas of science to give the audience a picture of what is happening today in physics.

a) Prof. Henry Glyde spoke on the latest results in disordered systems.

b) Prof. Vladimir Yarunin spoke on Bose-Einstein condensation in translation non-invariant systems.

c) Prof. Hubert Klar spoke on electron impact ionization of matter. This lecture gave the audience a window into atomic structures.

d) Dr. Wichit Sritrakool spoke on optical absorption in amorphous semiconductors.

e) the final physics speaker was Dr. David Sherwell who lectured on the mechanical origin of the second law of thermodynamics. This could be of great significance since many physicists are not satisfied with the current formulation of the foundations of Thermodynamics.

The final two lectures were of special interest to the mathematicians in the audience. Dr. Amnuay Kanantai lectured on how to solve the generalized wave equation in Euclidean Space and Dr. Suthep Suantai lectured on matrix transformations of vector-valued sequence spaces.

The lecture on the generalized wave equation was of great interest to the physics graduate students who had a long informal discussion with Amnuay about his techniques and results.

#### ***4) Attending Conferences and Workshops***

The fourth area listed concerned using TRF grant to support FTS staff members to attend conferences and workshops abroad so that they could learn from the world's leading experts and acquaint their colleagues with their latest ideas.

##### ***4.1 Mathematics***

4.1.1 Our FTS mathematics director, Dr. Sidney S. Mitchell, was able to attend a conference on Universal Algebra and Combinatorics at the University of Potsdam, Germany in June 1997 thanks to TRF support. He presented a paper entitled "Convex Algebra" which was well received and published in the proceedings.

4.1.2 In addition Dr. Mitchell, with TRF support, was able to go abroad attending the "International Congress on Algebra and Combinatorics" held at the Chinese University of Hong Kong during the month of August. While there he presented a paper entitled "Archimedean Ordered Semifields" which was published in the proceedings of the conference.

- 4.1.3 Finally, Dr. Mitchell received TRF support to attend two conferences in Thailand, "Universal Algebras and Semigroups" (3-5 March'98 at Khon Kaen University) and "The Workshop on General Algebra" (9-20 March'98) at Chiang Mai University).
- 4.1.4 There was a conference on algebraic analysis sponsored by FTS and held at Suranaree University from 26 January to 2 February, 1997. FTS covered all expenses for this conference, not only the speakers expenses but also the expenses of Drs. Pairoaj Satthaytham and Suwon Tangmanee who made many trips to Bangkok to confer on details needing to be settled in order for the conference to succeed.
- 4.1.5 Dr. Amnuay Kanantai's excellent research has been recognized outside of Thailand and he was invited to present his work at a mathematics conference in Belgium this August. FTS will enable *him to go by fully supporting his travel expenses and accommodation.*
- 4.1.6 Dr. Suthep Snantai will be supported by FTS to attend the conference "Function Spaces EMBED Equation" at Poland from 28 August to 2 September 1998. Dr. Suthep is one of the best young mathematicians who graduated from Chulalongkorn University. We are sure that he will gain a lot from the conference and contribute a lot to mathematics.

## 4.2 Physics

The staff of FTS's Physics section who received FTS support were the following:

- 4.2.1 Dr. Pornthep Nisamaneephong and Mr. Udom Robkob who visited the Seoul National University, Korea from 4-10 June 1996 to attend the "International Advisory Board Committee of the Inauguration Conference of the Asia Pacific Center for Theoretical Physics". We expect that they will be very active in all the future programs of the APCTP.

- 4.2.2 Mr. Porncharoen Palataidamkerng, M.Sc. Physics and a staff member of Chulalongkorn University, was supported by FTS and Vietnam on two occasions to attend "The Particles School" in Hanoi in October 1996 and "The Fifth School of Particle Physics, Quantum Field Theory and Applications" from 22 December 1997 to 3 January 1998 in Ho Chi Minh City.
- 4.2.3 The third person to receive traveling support was Mr. Kobchai Tayanasant who has a M.Sc. in Physics from Chulalongkorn University and is expected to have a brilliant future. He is currently a student sponsored by the Royal Golden Jubilee Ph.D. program studying at Department of Physics under the supervision of Prof. Virulh Sa-yakanit. He was supported by Vietnam and FTS to attend the same conference as Porncharoen in Ho Chi Minh City.
- 4.2.4 Mr. Klaus Hass of Ubon University made many visits to FTS to collaborate with Prof. Virulh Sa-yakanit. This collaboration led to two papers one published in the International Journal of Modern Physics and the other in Physical Review. One paper studied Electron Plasmon and the other paper applied path integration to the study of heavily doped semiconductors. Mr. Hass visited FTS for periods ranging from one week to three months. His travel expenses and his accommodation fees were all covered by FTS.
- 4.2.5 Dr. Nikom Choosiri a former Ph.D. graduate at FTS who is now working at Taksin University in Songkla is currently collaborating with Prof. Virulh Sa-yakanit on problems concerning the Quantum Hall Effect. Like Mr. Hass, his traveling expenses and his local expenses are being completely covered by FTS.

Finally, in recognition of his status as an international physicist, Prof. Virulh Sa-yakanit received many invitations to lecture at physics conferences around the world. FTS supported some of his expenses while his hosts provided the rest. Below is a list of the conferences he attended in the 1996-1998 period:

- 4.2.6 visited the Institute for Solid State Physics at the University of Tokyo to discuss SORTEC (Synchrotron Orbital Technology) with Prof. Ishii from 28 January to 3 February 1996.

- 4.2.7 visited KEK Tsukuba, Japan from 7-9 February 1996 to be a member of the fourth International Planning Committee for APCTP (Asia Pacific Center for Theoretical Physics).
- 4.2.8 visited Pohang University of Science and Technology in Pohang, Korea from 8-9 April 1996 to attend the First Asian Committee for Future Accelerators Meeting.
- 4.2.9 visited the "Dubna Joint Meeting of International Seminar Path Integrals : Theory and Applications" Conference on Path Integrals from meV to MeV" held in Dubna, Russia 27-31 May 1996.
- 4.2.10 visited the Asia Pacific Center for Theoretical Physics at the Seoul National University to be a member of the International Advisory Committee of the Inauguration Conference of the Asia Pacific Center for Theoretical Physics. Length of stay was 7 days, from 4-10 June 1996.
- 4.2.11 accompanied the Thai Physics Olympics team to Oslo, Norway from the end of June to the beginning of July 1996.
- 4.2.12 visited Beijing from 7-9 August 1996 to attend the "International Symposium on Climate and Global Environmental Changes.
- 4.2.13 visited San Francisco from 14-17 March 1997 to attend the "Seventh Annual Workshop on Science and Technology : Exchange Between Thai Professionals in North America and Thailand".
- 4.2.14 visited Kuala Lumpur, Malaysia from 9-11 July to attend the "International Conference on Frontiers of Quantum Physics".
- 4.2.15 visited Beijing to attend the General Ordinary Meeting and the Council Meeting of the Association of Asia Pacific Physical Societies (AAPPS) from 14-20 August 1997.
- 4.2.16 visited Tsukuba, Japan to attend the celebration for the combining of three Japanese high Energy Physics groups. The celebration took place on 16 September 1997.

- 4.2.17 visited Korea on 22 May 1998 to attend a General Council Meeting at the APCTP Center.
- 4.2.18 visited Paris, France from 27-29 May 1998 to attend the symposium entitled "Niels Bohr and the Evolution of Physics in the Twentieth Century".
- 4.2.19 will visit Florence, Italy from 25-29 August 1998 to present a plenary talk at the "Sixth International Conference on Path Integrals from peV to TeV : Fifty Years from Feynman's Paper".

### ***5) Foreign Experts***

The fifth area that we listed in our proposal concerned inviting foreign experts to visit FTS and do research with our staff. We are proud to say that we had more than thirty five visits from outstanding foreign researchers. We list the relevant data concerning these people below.

- 5.1 Prof. Helmut Wiedemann, a Professor from Stanford, SLAC gave a series of talk on acoustics physics in 1996.
- 5.2 Prof. Herman Winick, from Stanford, SLAC gave a talk on the Application of Synchrotron Radiation in 1996.
- 5.3 Prof. M. P. Das, from the Australian National University, gave a talk on Quantum Hall Effect in 1996.
- 5.4 Prof. Youyan Liu, a physicist from South China University of Technology, visited FTS as a researcher in 1996.
- 5.5 Prof. Lebohang K. Moleko a physicist currently with the Lesotho Embassy of China visited FTS as a researcher in 1996.
- 5.6 Prof. Vladimir Yarunin a physicist from the Joint Institute for Nuclear Research and the Bogoliubov Laboratory of Theoretical Physics in Russia visited FTS as a researcher in 1996.

- 5.7 Prof. Wolfgang Weller, a physicist from the University of Leipzig, Germany visited FTS as a researcher in 1996.
- 5.8 Prof. William B. Daniel, a physicist from University of Delaware in the U.S.A., visited FTS as a researcher in 1996.
- 5.9 Prof. John W. White, from the Australian National University, visited FTS and gave a talk on the X-ray Crystal Structure in the workshop on “Applications of Synchrotron Radiation”, 3-7 January 1996.
- 5.10 Dr. Vince C. Kempson, a physicist from Oxford Instruments, England, visited FTS and gave a talk on the Technology Involved in the Construction of Small and Medium Size Synchrotron Light Sources and Beamline Technology for Third Generation Light Sources, in the workshop on “Applications of Synchrotron Radiation”, 3-7 January 1996.
- 5.11 Prof. Antony Bourdillon, a physicist from National University of Singapore, Singapore, visited FTS and gave a talk on the X-ray Lithography in Singapore, in the workshop on “Applications of Synchrotron Radiation”, 3-7 January 1996.
- 5.12 Prof. Elliott Lieb, a visiting professor from Princeton University, U.S.A. visited FTS and gave a talk on the Exact Ground State Energy of the Strong-Coupling Polaron in 1996.
- 5.13 Prof. Leif Matsson, a visiting professor from Gothenberg University, Sweden visited FTS and gave a talk on the Biophysics and Medical Physics in January 1996.
- 5.14 Dr. Mikael Eriksson, a physicist from MAX LAB, Sweden, visited FTS and gave a talk on the Machine Design, visited FTS and participated in the workshop on “Applications of Synchrotron Radiation”, 3-7 January 1996.
- 5.15 Prof. Hiromichi Kamitsubo, a physicist from SPring-8 Project Team, Japan, visited FTS and gave a talk on the SPring-8 Project :

Status of the Construction, in the workshop on “Applications of Synchrotron Radiation”, 3-7 January 1996.

- 5.16 Prof. Motohiro Kihara, a physicist from the National Laboratory for High Energy Physics, Japan, visited FTS and gave a talk on the Development of the Photon Factory Storage Ring, in the workshop on “Applications of Synchrotron Radiation”, 3-7 January 1996.
- 5.17 Prof. Swee Ping Chia, a physicist from University of Malaya, Malaysia, visited FTS and participated in the workshop on “Applications of Synchrotron Radiation”, 3-7 January 1996.
- 5.18 Prof. S. C. Lim, a physicist from University Kebangsaan Malaysia,, Malaysia, visited FTS and participated in the workshop on “Applications of Synchrotron Radiation”, 3-7 January 1996.
- 5.19 Prof. Dao Vong Duc, a physicist from Vietnam National Institute of Physics, Vietnam, visited FTS and participated in the workshop on “Applications of Synchrotron Radiation”, 3-7 January 1996.
- 5.20 Prof. Nguyen Van Do, a physicist from Academy of Science of Vietnam, Vietnam, visited FTS and participated in the Workshop on “Applications of Synchrotron Radiation”, 3-7 January 1996.
- 5.21 Prof. Parangtopo Sutokusumo, a physicist from Graduate Study Programme of Science, University of Indonesia, Indonesia, visited FTS and participated in the workshop on “Applications of Synchrotron Radiation”, 3-7 January 1996.
- 5.22 Prof. Danilo M. Yanga, a physicist from University of the Philippines, Philippines, visited FTS and participated in the workshop on “Applications of Synchrotron Radiation”, 3-7 January 1996.
- 5.23 Prof. Krishna B. Garg, a physicist from University of Rajasthan, India, visited FTS and participated in the workshop on “Applications of Synchrotron Radiation”, 3-7 January 1996.

- 5.24 Prof. Shekhar Gurung, a physicist from Tribhuva University, Nepal, visited FTS and participated in the workshop on “Applications of Synchrotron Radiation”, 3-7 January 1996.
- 5.25 Prof. Taeyeon Lee, a physicist from Pohang Accelerator Laboratory POSTECH, Korea, visited FTS and participated in the workshop on “Applications of Synchrotron Radiation”, 3-7 January 1996.
- 5.26 Prof. Dieter Schuch, a physicist from Institute of Theoretical Physik, Frankfurt, Germany, visited FTS and gave a series of lectures on Irreversibility, Dissipation and Nonlinearity in Classical and Quantum Mechanics in April 1996.
- 5.27 Prof. Akito Arima Riken, a physicist working in Japan, visited FTS as a researcher in 1996.
- 5.28 Prof. Victor D. Lakhno, a mathematician from the Institute of Mathematical Problems in Biology, Russia, visited FTS to do research from 5 October-28 December 1996.
- 5.29 Mr. Klaus Hass a German physicist from Ubon Ratchatani University visited FTS to do research from 4 November-27 December 1996.
- 5.30 Dr. Gabriella Metodieva Slavtcheva, a physicist from the Institute of Biophysics of the Bulgarian Academy of Sciences, visited FTS to do research from 31 July 1997-31 January 1998.
- 5.31 Prof. Youyan Liu, a physicist from South China University of China, revisited FTS to do research from 1-31 August 1997.
- 5.32 Prof. A. Muriel, a physicist from the University of the Philippines at Los Banos, visited FTS to do research from 30 April-2 May 1998.
- 5.33 Prof. Xiang Xialin, a mathematician from Chengdu Universtiy in China, came to visit FTS to give a three day workshop from 27-29 April 1998 on applications of functional analysis to control theory.

- 5.34 Ms. Song Liyan a physicist working in China visited FTS to do research from 6 May-5 June 1998.
- 5.35 Dr. Hugo Christensen, a physicist from the Australian National University, visited FTS in July 1998.
- 5.36 Prof. Henry Glyde, a physicist from the University of Delaware, U.S.A., visited FTS to do research from 15-25 September 1998 and participated in the Third Meeting in Theoretical Physics : Feynman's Path Integrals and Theoretical Physics held at Chulalongkorn University on Thursday 17 September 1998.
- 5.37 Prof. Herbert Klar, a physicist at the Albert-Ludwigs-Universitat in Germany, will visit FTS to do research from 1 September-15 October 1998 and participated in the Third Meeting in Theoretical Physics : Feynman's Path Integrals and Theoretical Physics held at Chulalongkorn University on Thursday 17 September 1998.
- 5.38 Prof. Vladimir Yarunin mentioned above visited FTS to do research from 14-21 September 1998 and participated in the Third Meeting in Theoretical Physics : Feynman's Path Integrals and Theoretical Physics held at Chulalongkorn University on Thursday 17 September 1998.
- 5.39 Prof. Dao Vong Duc, a physicist from Vietnam National Institute of Physics, Vietnam, visited FTS to do research from 18 - 28 September, 1998.

## **6) Research on Feynman's Path Integrals**

The sixth area that we listed in our proposal concerned the number of graduate students who would finish their research by applying the Feynman Path Integral to such fields as disordered systems, the Quantum Hall Effect, polarons, plasmarons and wavelets. We are very happy to say that six students at FTS graduated from Chulalongkorn University. They are listed below.

- 6.1 Mr. Kobchai Tayanasant received his M.Sc. degree; his thesis is entitled "Effective Mass of the Polaron". Some of his thesis work

was published in Physical Review B. It is very rare for a master's degree student to publish results in such a prestigious journal.

- 6.2 Mr. Varagorn Piputnchonlathee received his M.Sc. degree; his thesis is entitled "Path Integral Approach to Heavily Doped Semiconductors : Two Variational Method". Part of this thesis was submitted to the Journal of Physics C, we expect it to be published. Varagorn is currently studying for his Ph.D. degree at the University of Manchester, England.
- 6.3 Ms. Sivinee Sawatdiaree received her M.Sc. degree; her thesis is entitled "Path Integral Approach to the Bose Condensation". She is currently studying at the University of Leipzig, Germany under the supervision of Prof. Wolfgang Weller.
- 6.4 Mr. Jessada Sukpitak received his M.Sc. degree; his thesis is entitled "Einstein Relation of Heavily Doped Semiconductors". He is now at FTS studying for his Ph.D. degree on optical absorption of amorphous semiconductors.
- 6.5 Mr. Santipong Boribarn received his M.Sc. degree; his thesis is entitled "Free Energy of a Particle with Saddle Point Potential in Magnetic Field".
- 6.6 Mr. Udom Robkob received his Ph.D. degree; his thesis is entitled "Path Integral Approach to Mobility". Mr. Udom Robkob was only the third person to receive his Ph.D. in physics from a Thai institution of higher education.

All the above mentioned scientists graduated in 1997.

## ***7) Recruiting Graduate Students***

The seventh area that we mentioned in our proposal concerned recruiting of students at the M.Sc. and Ph.D. levels who would be supported by FTS.

We have been very successful in this area. At the beginning of the 1996-1998 period we had one Ph.D. student and three M.Sc. students. We now have four Ph.D. students and five M.Sc. students. We list the students and their fields of research.

- 7.1 Mr. Kobchai Tayanasant is a Ph.D. student and he is studying the path integral approach to superfluids.
- 7.2 Mr. Teerawat Prakobpon is a Ph.D. student and he is studying heterostructures of semiconductors and superlattices. It is worthwhile to note that Tirawat's research is both theoretical and experimental. He has been conferring with engineers and he has done experiments in the engineering department.
- 7.3 Mr. Jessada Sukpitak is a Ph.D. student and he is studying optical absorption of amorphous semiconductors.
- 7.4 Mr. Prasopchai Viriyasrisuwattana is a Ph.D. student and he is studying path integral approach to polymers.
- 7.5 Mr. Supitch Khaemani is a M.Sc. student and he is studying flux line motion in superfluids.
- 7.6 Mr. Chatchawal Sripakdee is a M.Sc. student and he is studying the conductivity of metallic hydrogen.
- 7.7 Mr. Prathan Sreevilai is a M.Sc. student and he is studying tunneling in Schottky junction at low bias.
- 7.8 Mr. Sutee Boonchui is a M.Sc. student and he is studying geometric face in physics.
- 7.9 Mr. Suchat Kaskamalas is a M.Sc. student and he is studying the hydrodynamics of superfluids.

## **8) International Publications**

The eighth area that we listed in our proposal concerned publications in international journals of FTS papers. We said that we expected to publish at least one paper in an international journal. In fact we published eight physics papers in some of the most respected international journals in the world. We now list the papers.

### ***8.1 Published***

- 8.1.1 Sa-yakanit V., Lakhno V. D. and Hass K., "Path Integral Calculations of Particle Self-Energy and Effective Mass in Coulomb Systems", *Modern Physics Letters B*, Vol. 11, No. 4 (1997) 129-138.
- 8.1.2 Sa-yakanit V., "Path Integral and Variation Method in the Band Tail Problem", *Physics Letters A*, 240 (1998) 167-170.
- 8.1.3 Sa-yakanit V., Yarunin V. and Nisamaneephong P., "Bose-Einstein Condensation in Nonuniform Media", *Physics Letters A*, 237 (1998) 152-156.
- 8.1.4 Sa-yakanit V. and Tayanasanti K., "Consistent Definition of the Effective Mass of the Polaron", *Physics Review B*, Vol. 57, No. 15 (1998) 8739-8742.
- 8.1.5 Sa-yakanit V., Lakhno V. D. and Hass K., "Path Integral Approach to Single-Particle Excitation in Coulomb Systems", *Physics Review B*, Vol. 57, No. 10 (1998) 5772-5777.

### ***8.2 Accepted***

- 8.2.1 Sa-yakanit V. and Slavcheva G., "Path Integral Approach to the Electron Density of States at the Interface of a Single Modulation-Doped Heterojunction" accepted for publication by *Physical Review B*, 1998.
- 8.2.2 Kananthai A., "On the Fourier Transform of the Diamond Kernel of Marcel Riesz" accepted for publication by *Applied Mathematics and Computation* 1998.

### ***8.3 Submitted***

- 8.3.1 Natenapit M. and Sanglek W., "Capture Radius of Magnetic Particles in Random Cylindrical Matrices in High Gradient Magnetic Separation" submitted to the *Journal of Applied Physics*.

## **8.4 Proceedings**

- 8.4.1 Natenapit M., "Efficiency of High Gradient Magnetic Separation", Proceedings of the Third International Symposium of Eternet-Apr : Conservation of the Hydrospheric Environment, 3-4 December 1996, Chulalongkorn University, Bangkok, Thailand.
- 8.4.2 Sa-yakanit V., "A Model of Electron Transport in Solids : Path Integral Approach", Proceedings of the Dubna Joint Meeting of International Seminar Path Integrals : Theory and Applications and the Fifth International Conference Path Integrals from meV to MeV, Dubna 27-31 May 1996.
- 8.4.3 Sa-yakanit V. and Tayanasant K., "Static and Dynamic Effective Masses of the Polaron", p.256 in Frontiers in Quantum Physics (the Proceeding of the International Conference on Frontiers in Quantum Physics Kualalumpur, Malaysia, Editors: S. C. Lim, R. Adb-Shukor, and K. H. Kwek, Springer (1998).

## **8.5 Conferences**

- 8.5.1 Sa-yakanit V. and Boribarn S., "Path Integral Approach to the Landau Levitation in 2-D Random Systems", to be presented as a plenary talk at the "Sixth International Conference on Path Integrals from peV to TeV : Fifty Years from Feynman's Paper", held in Florence, Italy, 25-29 August 1998 .
- 8.5.2 Kananthai A., "A Survey of Distribution Theory in Solving Differential Equations", presented at ICCAM 98 Katholieke Universiteit Leuven, Belgium 27 July to 2 August 1998.
- 8.5.3 Suantai S., "Matrix Transformations of Some Vector Valued Sequence Spaces" to be presented at the International Conference on Function Spaces 28 August-3 September 1998, held at Poznan University of Technology in Poland.
- 8.5.4 Kananthai A., "On the Convolution Equation Related to the N-Dimensional Ultra-hyperbolic Operator" presented at the

### ***9) Inter-University Collaboration***

The ninth area that we listed in our proposal concerned FTS's in promoting a collaboration between Chulalongkorn University's mathematics department and the mathematics departments of Suranaree University of Technology.

We are happy to say that a new journal of mathematics in Thailand has been created, it is the first Thai journal of mathematics and the driving force behind this journal was Dr. Suwon Tangmanee of Suranaree University.

The staff of FTS has supported this journal strongly. We expect that our staff will referee submitted papers and we shall do our utmost to maintain the highest standard.

Dr. Pairoaj Satthaytham of Suranaree University promoted a three day FTS workshop at Chulalongkorn University from 27-29 April 1998 on "Applications of Functional Analysis to Control Theory". The speaker was Prof. Chiang Chiaolin from the University of Chengdu in Chian. Prof. Chiang was visiting Suranaree University for a three month teaching and research sabbatical and Dr. Pairoaj found her lectures so clear and profound that he contacted Dr. Mitchell, the director of the mathematics section, to have a workshop so that all Thai mathematicians could learn from Prof. Chiang.

We are very proud of our cooperative efforts with Suranaree University. However, again FTS surpassed its initial expectations. FTS has also sponsored a cooperative effort between the mathematics departments of Chulalongkorn University and Chiang Mai University. Three very active researchers on the staff of Chiang Mai University have been accepted as staff members of FTS's mathematics section. They are Dr. Amnuay Kananthai, Dr. Suthep Suantai and Dr. Vites Logani.

Drs. Amnuay and Suthep are both interested in Functional Analysis and Dr. Amnuay has set up a research group on "the integral transforms of operators" under the supervision of Prof. Virulh Sa-yakanit and FTS.

Dr. Vites' interests lie in combinatorics which complements the analysis of the other two.

## ***10) Concerning Thailand's Synchrotron Radiation***

The tenth area that was listed concerned FTS's involvement in solving some of the theoretical problems that may occur in constructing Thailand's synchrotron radiation machine.

Mr. Klaus Hass is on the staff of the physics department of Ubon University. He did his Master's degree on microwaves so it was very natural to choose him for advanced training in synchrotron radiation. Also he has published very good results with Prof. Virulh Sa-yakanit in international physics journals so he again was an obvious choice for the synchrotron radiation.

When Prof. Virulh Sa-yakanit was the head of the synchrotron radiation program, he sent Mr. Klaus Hass to Tsukuba, Japan, which is one of the world's leading centers in synchrotron radiation research, to learn the latest techniques and developments for the key physicists working on the Thailand synchrotron radiation program.

Of course, FTS and its director Prof. Virulh Sa-yakanit were responsible for creating the Thai synchrotron radiation program and also bringing the machine to Thailand. From 1996-1997 FTS was responsible for the training of Thai scientists in the use of the machine and the theoretical basis of synchrotron radiation.

## ***11) Concerning ICTP***

The eleventh area that we listed concerned cooperation with the International Centre for Theoretical Physics (ICTP) in Trieste, Italy. Our stated goals of maintaining our existing federation agreement and senior associate membership have been achieved. In each of the past three years ICTP has renewed our applications for maintaining our federation and senior associate membership.

ICTP has been encouraging all its associates to become established in their own countries and to try to depend on ICTP less and less. FTS has complied with ICTP's desire for its associates to be more independent. All the accomplishments listed above were done with only a little help from ICTP. The help that ICTP provided was the donation of scientific books which were useful references for our staff and students. However, during the past three years none of our staff or students visited ICTP although they continue to send us announcements of scientific meetings.

## ***12) Concerning APCTP***

The final area that we listed concerned FTS's relationship with the newly established Asia Pacific Centre for Theoretical Physics (APCTP) which was established in Korea in June 1996.

Prof. Virulh Sa-yakanit was made a member of the General Council because he was a founding member of APCTP. As a result, he sat in on the first inauguration of the APCTP with a young Thai physicist named Pornthep Nisamaneepong who was supported by FTS funds.

The APCTP is just beginning so right now it does not have many programs that FTS can be a part of. We are sure that this will change in the near future and with Prof. Virulh Sa-yakanit on the General Council, FTS will play a big part in these future programs.

## ***13) Concerning AAPPS and ASEANIP***

While talking of Asian organizations, we would like to mention that there is another important physics society, the Association of Asia Pacific Physical Societies (AAPPS) and Prof. Virulh Sa-yakanit also sits on their council and is a member of the editorial board of their journal. Again, Prof. Virulh Sa-yakanit will make sure that FTS will be a part of any programs of importance sponsored by the AAPPS in the future.

On the ASEAN region, Prof. Virulh Sa-yakanit currently serves as the President of the ASEAN Institute of Physics (ASEANIP). During his presidency, he has accepted Vietnam Institute of Physics as the sixth member. He also plans to invite Myanmar, Laos and Cambodia to join the ASEANIP in the future.

On the international role, he is also a member of the Third World Academy of Science (TWAS).

# ***APPENDIX 1***

(BRIEF SUMMARY)

**A Proposal for Upgrading the  
Forum for Theoretical Science FTS  
to be a Centre of Theoretical Sciences**  
(submitted to TRF at the beginning of the project)

(BRIEF SUMMARY)

**A Proposal for Upgrading the  
Forum for Theoretical Science FTS  
to be a Centre of Theoretical Sciences**  
(submitted to TRF at the beginning of the project)  
**by**

**Virulh Sa-yakanit**  
**Forum for Theoretical Science (FTS), Physics Department,**  
**Faculty of Science, Chulalongkorn University,**  
**Bangkok 10330, Thailand**

**Phone number: (66) (2) 251 7300, 218 5113, 218 5111**

**Telefax number : (66) (2) 255 2775**

**E-mail : svirulh@chula.ac.th**  
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**1. Introduction : Need for upgrading the FTS**

**1.1 Background**

FTS (Forum for Theoretical Science) was established at Chulalongkorn University in 1987 with Prof. Virulh Sa-yakanit as its current director. FTS has as its sole purpose the development of the basic sciences such as mathematics, physics, chemistry, biology, economics etc. in Thailand. From its inception, FTS has concentrated all of its energies and activities on developing mathematics and physics. These activities have been made possible over the last eight years by the generous support of Chulalongkorn University and International Centre of Theoretical Physics (ICTP). The fruits of that activity can be seen by the fact that FTS has produced several graduate students, one Ph.D. and twenty M.Sc. students in physics. In addition, approximately one hundred physicists and mathematicians from foreign countries have been able to visit here due to the support of FTS. Three physics conferences, bringing leading physicists from all over the world, were held at Chulalongkorn University under the auspices of FTS. Also, one International Conference on Geometry was sponsored by FTS.

These activities have brought great benefit to the staff members of both the mathematics and physics departments because they enabled the staff and

students to keep up with the most recent developments in mathematics and physics.

However, FTS cannot encourage or build up the student manpower outside of Chulalongkorn University. In order for FTS to be able to expand the opportunities of staff and students outside of Chulalongkorn University, it is necessary for FTS to grow and increase its activities. FTS must do more than just grow, it must become a center of excellence in Thailand where the most challenging ideas in the main stream of physics and mathematics are being investigated. To accomplish this, FTS needs the resources to enable it to invite experts from abroad to come and teach the latest developments at the frontiers of research. FTS envisions inviting visiting professors, experts and postdoctoral students for both short term and long term stays. Such a scheme should create a very challenging atmosphere for all Thai physicists and mathematicians to be motivated to achieve their full potential. With this kind of stimulation and support all around them, we expect to be able to train enough good young students and scientists to fulfill the needs of the country as we face a very competitive future. We are convinced that we can make a significant start in training the excellent young scientists that Thailand's future so desperately needs to be a great benefit to our country.

## **1.2 Need for Upgrading FTS**

Physics, Mathematics, Chemistry and Biology form the basis of other science based subjects such as engineering, medicine, materials science, agriculture, metallurgy, economics and a wide spectrum of other fields. In the past fifteen to twenty years, engineering and medicine have made great progress in Thailand. Many excellent engineers and medical doctors have been trained abroad and in Thailand and are in full practice today. By comparison, the more basic sciences lag far behind. Indeed, they lag so far behind that the level of basic sciences taught to engineers in Thai universities may limit their ultimate potential. There is a great need to promote the basic sciences in order to redress this imbalance. In today's climate of support for research and education, it is more difficult to make a case for the basic sciences. The returns are more diffuse and on a longer time perspective. Yet the need for strength in the basic sciences is very real, if only as a foundation for engineering, medicine, economics etc. viewed as a whole.

## **1.3 The National Need-Thailand**

Thailand has developed dramatically in the past 20 years with gross domestic product expanding 8-10 % annually. This has been based on a diligent and inexpensive labor force who have made several industries outstanding successes such as textiles, leather goods, clothing manufacture and assembly of electronic goods. Thailand has also excelled in medicine, engineering and agriculture as well as tourism.

This success and improvement in living standards brings new challenges. Compared to Vietnam, Bangladesh and the other now less developed nations, labor costs are no longer cheap here in Thailand. Labor intensive manufacture is moving away from Thailand to other nations. To continue economic progress, Thailand must bring technological innovation to the manufacturing process. This requires skilled manpower educated in science and technology.

While Thailand has excelled in engineering and medicine, it remains undeveloped in mathematics and physicals on which new technology and innovation are ultimately based. In Thailand, a nation of 60 million people and an undergraduate student population of approximately a quarter of a million, there are 25 Ph.D.'s. in mathematics and 125 in physics. To continue improvement in living standards, Thailand now seeks to develop the basic sciences. This new scientific base must also become and remain integration with the international community in mathematics and physics. This integration will bring a continual flow of ideas and techniques to Thailand so that modern education in mathematics and physics can be sustained and new technology can be used at an early stage of development.

## 2. Objectives

The main objective is to develop highly qualified manpower in physics and Mathematics in Thailand. Firstly, there is a need to develop and sustain an active interest in fundamental physics, mathematics and modeling in the scientific community of Thailand. Those people currently interested need support both for their individual research and for their interaction with others equally interested. Secondly, it is vital to attract some of the young students into Theoretical Science to provide excitement for them in their research so that they can be active and stimulating advocates of their science. In detail, we can summarize the situation:

- 1) To foster advanced research in Theoretical Physics and Mathematics.
- 2) To provide a center and focus for cooperation between individuals and groups in the above disciplines.

- 3) To provide facilities and space for individuals to conduct their research.
- 4) To organize lectures, seminars, group discussions and in particular to attract speakers from the international scientific community for short and longer term visits.
- 5) To assist young researchers and graduate students in Thailand to develop their full capabilities.
- 6) To serve as a model institute for basic sciences in the country.

### 3. Action Plan to Upgrade FTS

In order for FTS to become an internationally recognized center of excellence we need several things. We need to upgrade the knowledge technologies of FTS to the state of the art so that we can have instant notification of the latest major discoveries in science. Also, we need an up to date library so that we can understand the latest problems that the world's greatest scientists are working on. Of course we need good working conditions so that first class scientists will be willing to come and teach us and young Thai science students will desire to join us.

Also, in order to upgrade FTS we need to develop a whole new generation of gifted young Thai science students whose science background is @P an international standard and who are working together among themselves as well as working with outstanding scientists abroad in an international scientific link of people working on the same important scientific problems. This extended cooperation should be national, regional and international.

To achieve these goals, we propose the following courses of action:

- 1) We propose to have regular seminars with local scientists and visiting scientists from abroad so that we can have personal discussions to gain a clearer understanding of the latest happening in physics.
- 2) We propose to have annual meetings where large numbers of outstanding scientists can come to present their latest research and interact with each other to expand their ideas and gain deeper understanding.
- 3) We propose a continuous upgrading of our staff members and our graduate students through regular training in the new areas of science just opening up.

- 4) We propose a linkage program between Thai scientists and scientists throughout the world, especially the developed world.
- 5) We propose a newsletter to keep informed all the world's scientists of FTS's programs and progress.
- 6) We propose to develop collaborative research programs which simulate research at Thai universities for those Thai scholars who are just returning from abroad.
- 7) We propose to continue carrying on research in the field of Feynman Path Integrals. The path integral approach has wide and diverse application in a variety of scientific disciplines. The utility of path integrals is a standard practice for general studies in high energy physics. Path integrals have also proven to be effective tools in solving other problems, particularly in the low and intermediate energy range in such fields as (1) atomic and molecular physics, (2) chemical, polymer and reaction-rate physics, (3) statistical mechanics, (4) condensed matter physics, (5) nuclear physics, and (6) classical physics of waves (see appendix).

#### **4. Expectations for the Next Three Years**

- 1) We expect to have fully upgraded FTS's Mathematics and Physics sections. For example, we envision subscribing to the top quality mainstream journals in both mathematics and physics. These journals will be made available to the staff, students and visiting scholars of FTS. We also shall purchase the latest books in mathematics and physics which deal with mainstream themes. This is very important for the members of FTS because books are the way that a scientist is introduced to a new friend of science. Journal papers are written for those already expert in an area and are difficult, if not impossible, to be read by someone who wishes to join in researching a new area. Journal articles are extremely useful for those who have been properly introduced to a field. We also expect to expand our computer facilities to include Internet so that scientists can be involved in a day to day on going dialogue with all the other scientists in their fields of interest.
- 2) We hope to have a regular weekly general seminar once a week where FTS scientists can tell the other members of new results that they have discovered or of new results that they have learned from

outside scientists through Internet, journals etc. We intend to also organize a regular weekly special seminar where scientists of similar interests can discuss together what they already know, what new problems have been posed, where they would like to progress etc.

- 3) We plan to have regular annual meetings in both mathematics and physics. The topics of the meeting should be selected topics of current interest such as High Temperature Superconductivity, Quantum Hall Problem, Bose-Einstein Condensation, Bipolaron. Theory of Heavy Doped Semiconductor, Synchrotron Radiation, Analysis, Fuzzy mathematics, Geometry, etc.
- 4) We intend to financially support FTS staff members to visit conferences abroad, workshops at ICTP and fellow foreign scientists with the same interest.
- 5) Finally we intend to invite outstanding experts to come to FTS for either short term or long term visits to teach us the latest knowledge of their fields of expertise by presenting seminars or conferring personally with FTS scientists in their field.
- 6) We expect to have one or two graduate students finish their research work on the study of the applications of path integrals to quantum mechanics, more specifically to disordered systems, Quantum Hall, polarons, plasmarons and wavelets.
- 7) We hope to recruit more Master's and Ph.D. students to FTS whose work will be support by FTS.
- 8) We expect that in the next three years FTS will produce at least one international standard paper to be published in a widely read well respected international journal.
- 9) We intend to start a collaboration between Chulalongkorn University's Mathematics Department with FTS's theoretical physics group and other theoretical physics groups in Thailand such as Suranaree University.

- 10) We hope to play a part in solving some of the theoretical physics problems that may arise in the construction of Thailand's Synchrotron Radiation facility such as theoretical beam dynamics.
- 11) We hope to continue cooperation with the International Centre for Theoretical Physics by maintaining our existing Federation Agreement and Associate Member scheme. Also, we expect to continue the use of their existing facilities as we have done in the past.
- 12) We intend to support the newly established Asia-Pacific Centre for Theoretical Physics which will be established in Korea. It has the strong support of all Asian countries and promises to be a very important Centre of Excellence in Theoretical Physics in regional. We expect that FTS will have a mutually fruitful interaction with this centre.

## ***APPENDIX 2***

### **Papers Published in International Journals**

# Path-integral approach to single-particle excitation in Coulomb systems

V. Sa-yakanit, V. D. Lakhno,\* and K. Hass†

Forum for Theoretical Science, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

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The electron-plasmon Fröhlich-type Hamiltonian, introduced by Lundquist, is formulated in terms of the Feynman and the Luttinger-Lu generalized path-integral approach. It is shown that the average propagator for the plasmaron, the dressing of the electron by plasmons, can be evaluated by using both approaches. The average propagator is then used to obtain the ground-state energy for the plasmaron. It is shown that the Luttinger-Lu approach gives higher ground-state energies than those obtained by the Feynman approach for intermediate values of the coupling constant and lower for the strong-coupling limit.

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## I. INTRODUCTION

Progress in many-particle problems is generally associated with a successful model approach. In recent years, there have been intense research efforts on one-particle self-consistent treatments of many-particle systems.<sup>1,2</sup> In the case of a charged test particle interacting with an electron gas, the single-particle spectrum was investigated in an approximation with a particle coupled to plasmons.

A good example of such an approach in dielectrics is given by the theory of electronic polarons.<sup>3,4</sup> In this case, the electron-plasmon interaction of an electron in an empty conduction band and filled valence band leads to the renormalization of the electron mass and its energy similar to the case of polarons in ionic crystals. In metals, the one-particle treatment of an electron gas leads to the notion of plasmarons introduced by Lundquist working as an electron coupled to plasmons.<sup>5,6</sup> The electron-phonon coupling in metal leads to peculiarities in the single-particle spectrum and the existence of a tail of the density level at the bottom of the conduction band. This approach was also used by Overhauser<sup>19</sup> for the calculation of an exchange and correlation energy of the electron gas in metal.

In a semiconductor, electrons, surrounded by a cloud of screening holes in the conduction band of a *p*-type semiconductor and holes, and surrounded by a cloud of screening electrons in the valence band of an *n*-type semiconductor, were named continuum excitons.<sup>7</sup> The continuum-exciton theory based on electron-plasmon interactions was developed in Ref. 8.

In this work, a path-integral approach that describes the particle coupled with plasmons is developed. For metals, the path integral method was developed in Ref. 9 and for semiconductors in Ref. 10. As was demonstrated by Feynman,<sup>11</sup> the path-integral approach gives the best results for intermediate values of the coupling interaction in the case of electron-phonon coupling. This case is usually realized in the real system mentioned above, where the electron-plasmon interaction gives the main input at intermediate values of the coupling constant.

This paper is organized as follows: In Sec. II, we present the different expressions for the interaction of charged particles with plasmons in a dielectric, metal, and

semiconductor. It is significant that in all cases the interaction can be described by a Fröhlich-type Hamiltonian.

In Sec. III, we apply the Feynman approach, where the exact action is substituted by a probe action which has a harmonic form. For the case of electron-plasmon interactions in metals, the average propagator for the dressing of an electron by plasmon is evaluated. The averaged propagator is then used to obtain the ground-state energy of the electron at the bottom of the band. Both cases of weak and strong coupling are considered in Sec. IV.

In Sec. V, we develop the generalized path-integral approach and get the ground-state energy of a charged probe particle in an electron gas. The results obtained by this approach are compared with those obtained by the Feynman method in Sec. IV.

## II. ELECTRON-PLASMON INTERACTION IN DIFFERENT CASES

The system composed of one nonrelativistic particle interacting with a quantum field in the most general form of an interaction that is linear in the field operator is described by the Hamiltonian

$$H = \frac{p^2}{2m} + \sum_k C_k (b_k + b_k^\dagger) e^{ikr} + \sum_k \hbar \omega_k b_k^\dagger b_k, \quad (1)$$

where  $b_k^\dagger$  and  $b_k$  are the field operators of creation and annihilation,  $\omega_k$  are the field frequencies,  $C_k$  are the constants which characterized the interaction of particle and field, and  $m$  is the mass of the particle.

In the case of an excess electron in a dielectric, which interacts with plasmons of the valence band, the values of  $C_k$  and  $\omega_k$  are<sup>4</sup>

$$C_k = i \sqrt{\frac{2\pi e}{\epsilon V k}} \frac{\omega_p}{\sqrt{\omega_k}}, \quad \omega_k^2 = \omega_p^2 + \Delta_k^2, \quad \hbar \Delta_k = \hbar \Delta_0 + \frac{\hbar^2 k^2}{2m}, \quad (2)$$

where  $\omega_p = \sqrt{4\pi e^2 n_0 / m \epsilon}$  is the plasma frequency,  $e$  the electron charge,  $\epsilon$  the static dielectric permittivity,  $V$  the

volume of system, and  $\hbar\Delta_0$  equals the width of the gap in the dielectric. In the case of a semiconductor,<sup>8</sup>

$$C_k = i \frac{e}{k} \sqrt{\frac{2\pi}{\varepsilon V}} \left( \frac{\varepsilon(k)-1}{\varepsilon(k)} \right)^{1/4}, \quad (3)$$

where  $\varepsilon(k)$  is the static dielectric permittivity of the semiconductor. In the case of metal,<sup>5,6</sup>

$$C_k = i \frac{e}{k} \sqrt{\frac{4\pi\hbar}{V(\partial\varepsilon(\omega, k)\partial\omega)_{\omega=\omega_p}}}, \quad (4)$$

where  $\varepsilon(\omega, k)$  is the dielectric function. The dispersion law is taken as

$$\omega^2(k) = \omega_p^2 + \frac{1}{3} \left( \frac{\hbar k_F}{m} \right)^2 k^2 + \left( \frac{\hbar k^2}{2m} \right)^2. \quad (5)$$

### III. FEYNMAN APPROACH

To carry out the path integral for the propagator  $G(\mathbf{r}'', \mathbf{r}'; t)$ , which is given by the Feynman path-integral formalism by

$$G(\mathbf{r}'', \mathbf{r}'; t) = \int_{\mathbf{r}'}^{\mathbf{r}''} D[\mathbf{r}(\tau)] e^{iS/\hbar}, \quad (6)$$

where  $S$  is given by

$$S = \int_0^t \frac{m}{2} \dot{\mathbf{r}}^2(\tau) d\tau + \frac{1}{16\pi^2} \int d^3k C_k^2 \int_0^t \int_0^t d\tau d\sigma \times \frac{\cos[\omega_k(t/2 - |\tau - \sigma|)]}{\sin(\omega_k t/2)} e^{ik[\mathbf{r}(\tau) - \mathbf{r}(\sigma)]}. \quad (7)$$

We follow the Feynman method by the introduction of a trial action,<sup>9,12</sup> defined as

$$S_0(k, \Omega) = \int_0^t d\tau \left[ \frac{m}{2} \dot{\mathbf{r}}^2 - \frac{1}{8} \kappa \Omega \int_0^t d\sigma \left| \mathbf{r}(\tau) - \mathbf{r}(\sigma) \right|^2 \frac{\cos[\Omega(t/2 - |\tau - \sigma|)]}{\sin(\Omega t/2)} \right], \quad (8)$$

where  $\kappa$  and  $\Omega$  are parameters to be determined. The test-particle propagator  $G(\mathbf{r}'', \mathbf{r}'; t)$  can be rewritten as

$$G(\mathbf{r}'', \mathbf{r}'; t) = G_0(\mathbf{r}'', \mathbf{r}'; t) \left\langle \exp \left[ \frac{i}{\hbar} (S - S_0) \right] \right\rangle_{S_0}, \quad (9)$$

and the average over  $S_0$ ,  $\langle O \rangle_{S_0}$  defined by

$$\langle O \rangle_{S_0} = \frac{\int D[\mathbf{r}(\tau)] O \exp[(i/\hbar) S_0]}{\int D[\mathbf{r}(\tau)] \exp[(i/\hbar) S_0]}. \quad (10)$$

By approximating  $G(\mathbf{r}'', \mathbf{r}'; t)$  to the first cumulant, we obtain the approximate propagator  $G_1(\mathbf{r}'', \mathbf{r}'; t)$  as

$$G_1(\mathbf{r}'', \mathbf{r}'; t) = G_0(\mathbf{r}'', \mathbf{r}'; t) \exp \left[ \frac{i}{\hbar} \langle S - S_0 \rangle_{S_0} \right]. \quad (11)$$

The propagator  $G_1$  can be obtained if one can calculate  $G_0$  and  $\langle S - S_0 \rangle_{S_0}$ . This can be achieved by using the generating functional derived by Sayakanit.<sup>12</sup> This result for the diagonal part of  $G_1(\mathbf{r}'', \mathbf{r}'; t)$  is

$$G_1(0, 0; t) = \left[ \frac{mE_F}{2\pi i \hbar^2 t} \right]^{3/2} \left[ \frac{E_\nu \sin(E_\Omega t/2)}{E_\Omega \sin(E_\nu t/2)} \right]^3 \exp \left[ \frac{3}{2} \left( 1 - \frac{E_\Omega^2}{E_\nu^2} \right) \times \left( \frac{E_\nu t}{2} \cot \frac{E_\nu t}{2} - 1 \right) \right] + i C r_s^2 \int_0^\infty \frac{dE(k)}{\sqrt{E(k)} E_\omega(k)} \times \int_0^t ds (t-s) F'(E_\nu, E_\Omega, s), \quad (12)$$

where

$$F'(E_\nu, E_\Omega, s) = \frac{\cos[E_\omega(k)(t/2 - s)]}{\sin[E_\omega(k)t/2]} \times \exp \left[ -iE(k) \left( 1 - \frac{E_\Omega^2}{E_\nu^2} \right) \right] \times \left[ \left( \frac{E_\Omega^2}{E_\nu^2 - E_\Omega^2} \right) \frac{s}{t} (t-s) + \frac{2 \sin(E_\nu s/2) \sin[E_\nu(t-s)/2]}{E_\nu \sin(E_\nu t/2)} \right] \quad (13)$$

and we use the relations

$$E_\omega(k) = \sqrt{E_p^2 + \frac{4}{3} E(k) + E^2(k)},$$

$$E_F = (9\pi/4)^{2/3} r_s^{-2}, \quad E_p = \sqrt{12} \left( \frac{4}{9\pi} \right)^{2/3} r_s^{1/2},$$

$$E_p^2 \sqrt{\frac{E_F}{E_p}} = C r_s^2, \quad C = 12/\pi (9\pi/4)^{-5/3}, \quad (14)$$

where  $r_s = (9\pi/4)^{1/3} (1/k_F a_0)$ ,  $k_F$  is the Fermi wave vector,  $a_0$  the Bohr radius, and  $E_\Omega$  and  $E_\nu$  are parameters to be determined. The propagator  $G_1(0, 0; t)$  in Eq. (12) can be used to obtain various physical quantities such as the ground-state energy, the effective mass, the density of state, etc.

### IV. GROUND-STATE ENERGY IN THE FEYNMAN APPROACH

The ground-state energy can be obtained by letting  $t$  in Eq. (12) go to infinity. In this case, the approximate propagator can be expanded as a power series of the wave functions, having the ground-state term as its dominant term. Therefore,

$$G_1(0, 0; t) \cong u_0^*(0) u_0(0) e^{-iE_0' t}, \quad (15)$$

where  $E'_0$  is the ground-state energy measured in the unit of  $E_F$  and  $u_0(x)$  is the ground-state wave function. From Eqs. (12) and (15) we get

$$E'_0 = \frac{3}{4} E_\nu (1-\rho)^2 - Cr_s^2 \int_0^\infty \frac{dE(k) e^{\beta} \beta^{-\mu} \gamma(\mu, \beta)}{\sqrt{E(k)} E_\omega(k) E_\nu}, \quad (16)$$

where

$$\rho = \frac{E_\Omega}{E_\nu}, \quad \beta = -E(k)(1-\rho^2)/E_\nu,$$

$$\mu = (1/E_\nu)[E_\omega(k) + E(k)\rho^2],$$

and  $\gamma(\mu, \beta)$  is the incomplete gamma function. To obtain the best approximation for the actual ground-state energy, the two parameters  $\rho$  and  $E_\nu$  have to be varied separately to yield the minimum of  $E'_0$ . Below, we consider the asymptotic cases.

#### A. Weak-coupling limit

In the case of weak coupling  $r_s \rightarrow 0$ , we have  $\rho \approx 1$ . It is reasonable to set  $\rho = 1 - \varepsilon$ , where  $\varepsilon$  is a small parameter. From Eq. (16), expanding the incomplete  $\gamma$  function in terms of a series representation<sup>13</sup> and treating  $\beta$  as a small parameter, we obtain

$$E'_0 = \frac{3}{4} E_\nu \varepsilon^2 - Cr_s^2 \int_0^\infty \frac{dE}{\sqrt{E(k)} E_\omega(k) E'_\omega(k)} \times \left( 1 + \frac{2E(k)E_\nu \varepsilon}{E'_\omega(k)(E'_\omega(k) + E_\nu)} \right), \quad (17)$$

where  $E'_\omega = E_\omega(k) + E(k)$ . Differentiating the above equation with respect to  $\varepsilon$  and assuming as in Ref. 9

$$E'_\omega = \sqrt{E_p^2 + E^2(k)}, \quad (18)$$

we get

$$\varepsilon = \frac{4}{3} Cr_s^2 \int_0^\infty \frac{\sqrt{E(k)} dE(k)}{E_\omega(k) E_\omega'^2 [E'_\omega(k) + E_\nu]}. \quad (19)$$

Furthermore, in the considered limit we have  $E_p \gg E_\nu$ . Thus  $E_\nu$  in Eq. (19) may be neglected. Differentiating Eq. (17) with respect to  $E_\nu$  and expanding the result in a series leads to the following result for the ground-state energy:

$$E'_0 = \frac{3}{4} E_\nu \varepsilon^2 - \frac{Cr_s^2}{\sqrt{2}} E_p^{-3/2} B\left(\frac{1}{2}, \frac{3}{4}\right), \quad (20)$$

where  $B$  is the  $\beta$  function. In this limit of  $r_s \rightarrow 0$ , the leading term in Eq. (20) gives, for the ground-state energy  $E_0 = E_F E'_0$ ,

$$E_0 = -0.99 \frac{1}{r_s^{3/4}} \text{ Ry}, \quad (21)$$

where  $\text{Ry} = me^4/2\hbar^2$  is the Rydberg constant.

#### B. Strong-coupling limit

In this case  $\rho$  is small and can be approximated by zero. If we choose in this case the dispersion law as

$$E_\omega(k) \approx E_p, \quad (22)$$

we obtain the leading term in the energy  $E'_0$  in the form

$$E'_0 = \frac{3}{4} E_\nu - \frac{Cr_s^2 \pi \sqrt{\xi} \Gamma(\xi)}{E_p^{3/2} \Gamma(\xi + \frac{1}{2})}, \quad (23)$$

where  $\xi = E_p/E_\nu$ . In the limit  $E_\nu \rightarrow \infty$ , Eq. (23) leads to the following approximation:

$$E_0 = -0.106 + \frac{\text{const}}{r_s^2} \text{ Ry}. \quad (24)$$

Figures 1 and 2 show the graphics of the minima of Eq. (17), normalized to  $E_F$ , with  $\varepsilon$  given by Eq. (19) (dash lines). The dotted lines show the strong-coupling limit, given by the minima of Eq. (23). Figure 1 shows the results for a large range of  $r_s$ , while in Fig. 2, the range is restricted to  $r_s \in (1.5, 6)$ , which is appropriate for metals. In the next section, we compare this result with the Luttinger-Lu approach.

#### V. GENERALIZED PATH-INTEGRAL APPROACH

In order to apply the generalized path-integral approach to the considered system, we turn to the complex time  $t'' - t' = -i\beta\hbar$ . Following the Feynman path-integral formalism,<sup>14</sup> we obtain the density matrix  $\rho(r'', r'; \beta)$ , which depends only on the particle coordinates. The obtained density matrix leads to the expression for the ground-state energy of the considered system. Thus according to Eqs. (6) and (7), the ground-state energy  $E_l$  is equal to

$$E_l = -\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \ln \int_{r'(0)}^{r(\beta)} D[r(\tau)] e^{-S[r]}, \quad (25)$$

where

$$S[r] = \frac{m}{2} \int_0^\beta d\tau \dot{r}^2(\tau) + V(r), \quad (26)$$

$$V(r) = -2 \sum_k |C_k|^2 \int_0^\beta d\tau \int_0^\tau d\sigma e^{-|\tau-\sigma|\omega_k + i\phi[r(\tau) - r(\sigma)]}. \quad (27)$$

The upper limit of the ground-state energy  $E_l$  is determined by the Jensen inequality

$$E_l \leq \varepsilon_0 + \lim_{\beta \rightarrow \infty} \langle V - V_0 \rangle_{\varepsilon_0}, \quad (28)$$

where

$$\varepsilon_0 = -\lim_{\beta \rightarrow \infty} \int_{r'(0)=r(\beta)}^{r(0)=r'(\beta)} \int_{r'(0)=r'(\beta)} D[r(\tau)] D[r'(\tau)] e^{-S_0[r, r']} \times D[r(\tau)] D[r'(\tau)] e^{-S_0[r, r']}. \quad (29)$$

Note that the calculation of the ground-state energy with the use of the Jensen inequality (28) is equivalent to the calcu-

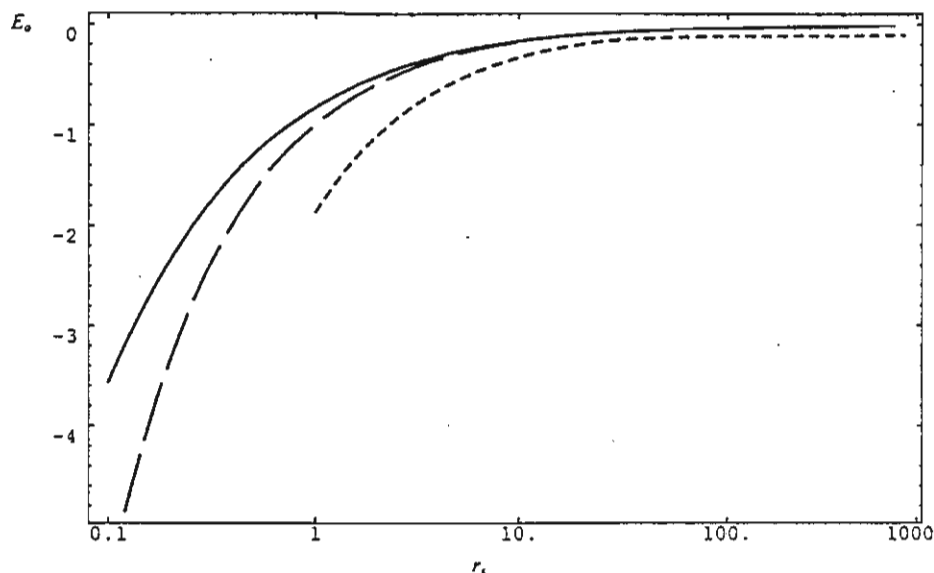


FIG. 1. The ground-state energy in the generalized path-integral approach (solid line), the weak-coupling limit (dashed line), and the strong-coupling limit (dotted line) of the Feynman approach.

lation of the first-order cumulant in expression (11). According to the generalized path-integral method,<sup>15</sup>

$$\varepsilon_0 - \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \langle V_0 \rangle_{S_0} = -\frac{1}{2\mu} \int d^3x u_0^*(x) \Delta u_0(x), \quad (30)$$

where  $u_0(x)$  is the wave function of the ground state for the Hamiltonian  $H_0$ , given by

$$H_0 = -\frac{1}{2\mu} \Delta + v_0(x). \quad (31)$$

Note that we set the mass of the particle equal to unity here. Thus the reduced mass  $\mu$  becomes  $M/(1+M)$ , where  $M$  is the fictitious mass to be determined. Using the same technique as in Ref. 15, we obtain, for  $\langle V \rangle_{S_0}$ ,

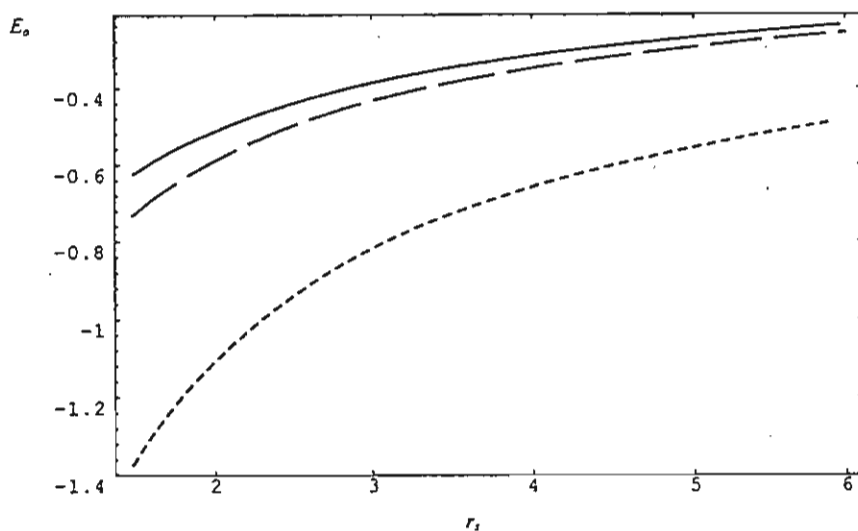


FIG. 2. The ground-state energy in the generalized path-integral approach (solid line), the weak-coupling limit (dashed line), and the strong-coupling limit (dotted line) of the Feynman approach in a range appropriate for metals.

$$\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \langle V \rangle_{S_0} = - \sum_k |C_k|^2 \int_0^\infty d\tau e^{-\omega_k \tau} e^{-k^2 \tau / 2(1+M)} \sum_{n=0}^\infty e^{-(\varepsilon_n - \varepsilon_0) \tau} \int u_0^*(x_1) u_n(x_1) u_n^*(x_2) u_0(x_2) e^{i\mu k(x_1 - x_2)} d^3 x_1 d^3 x_2. \quad (32)$$

Using Eqs. (28), (30), and (32), we obtain, for the upper bound  $E_0$  of the total energy  $E_I$ ,

$$E_I \leq E_0. \quad (33)$$

$$E_0 = \frac{1}{2\mu} \int |\nabla u_0|^2 d^3 x - \sum_k \frac{|C_k|^2}{\omega_k + k^2/2(1+M)} \left| \int |u_0(x)|^2 e^{i\mu k x} d^3 x \right|^2 - \sum_{n=1}^\infty \sum_k \frac{|C_k|^2}{\omega_k + k^2/2(1+M) + \Delta \varepsilon_n} \times \int u_0^*(x_1) u_n(x_1) u_n^*(x_2) u_0(x_2) e^{i\mu k(x_1 - x_2)} d^3 x_1 d^3 x_2, \quad (34)$$

where

$$\Delta \varepsilon_n = \varepsilon_n - \varepsilon_0 \geq 0. \quad (35)$$

Formulas (33)–(35) give the general expressions for the ground-state energy of the quasiparticle described by the Hamiltonian (1). The exact calculation of Eqs. (33)–(35) is too difficult and requires the solution of the nonlinear equation (31) and the equation for the minimization of  $E_0$ :

$$\frac{\partial E_0}{\partial \mu} = 0. \quad (36)$$

For an estimation of Eq. (34), we neglect the terms for  $n > 1$ . Thus we make inequality (33) even stronger. For  $u_0(x)$ , we choose the Gauss probe wave function

$$u_0(x) = \frac{l^{3/2}}{\pi^{3/4}} \exp\left(-\frac{l^2 x^2}{2}\right). \quad (37)$$

Using the relation  $\hbar \omega_p = \sqrt{12} r_s^{-3/2} \text{ Ry}$  and  $r_s = (9\pi/4)^{1/3} (1/k_F a_0)$ , where  $a_0$  is the Bohr radius, we obtain

$$E_0 = \frac{3}{2\mu} B^2 - \frac{2}{\pi} \sqrt[4]{12} r_s^{-3/4} \int_0^\infty dx \frac{\exp[-\sqrt{3} r_s^{-3/2} \mu^2 (x^2/B^2)]}{\sqrt{1 + (\pi^{2/3}/\sqrt{3}) \sqrt{2} \sqrt{r_s} x^2 + x^4}} \frac{1}{\sqrt{1 + (\pi^{2/3}/\sqrt{3}) \sqrt{2} \sqrt{r_s} x^2 + x^4 + (1-\mu)x^2}} \text{ Ry}, \quad (38)$$

where  $B = l a_0$ . The minima of Eq. (38) with respect to  $\mu$  and  $B$  are shown in Figs. 1 and 2 (solid lines). For more details, see Ref. 16.

#### A. Weak-coupling limit

In the case of the weak-coupling limit, when  $\mu \rightarrow 0$ , we get, from Eq. (34),

$$E_0 = - \sum_k \frac{|C_k|^2}{\omega_k + k^2/2}. \quad (39)$$

If we insert in Eq. (39) the dispersion law of formula (18) and  $C_k$ , defined by Eq. (4), we get

$$E_0 = -2 \frac{\sqrt[4]{12}}{\pi} I \frac{1}{r_s^{3/4}} \text{ Ry} = -1.0984 \frac{1}{r_s^{3/4}} \text{ Ry}, \quad (40)$$

where

$$I = \int_0^\infty dx \frac{1}{\sqrt{1+x^4}(x^2 + \sqrt{1+x^4})} = 0.927037. \quad (41)$$

The comparison with the result (21) shows that the generalized path-integral approach gives the ground-state energy, which is about 10% lower than that obtained by the Feynman

approach. However, in Fig. 1, the Feynman approach has lower energies in this limit. This is due to the fact that the convergence in the Feynman approach to Eq. (21) is much faster than in the generalized path-integral approach to Eq. (40).

#### B. Strong-coupling limit

In this limit,  $\mu \rightarrow 1$  and we have, from Eq. (34),

$$E_0 = \frac{1}{2} \int |\nabla u_0|^2 d^3 x - \sum_k \frac{|C_k|^2}{\omega_k} \left| \int |u_0(x)|^2 e^{i\mu k x} d^3 x \right|^2. \quad (42)$$

If we choose the dispersion law for  $\omega_k$  in the form (22), we obtain, from Eq. (42),

$$E_0 = -0.1085 \text{ Ry}. \quad (43)$$

This value coincides with the result of the strong electron coupling with optical phonons in the polaron theory<sup>17,18</sup> and can be compared with the result of Eq. (24). The difference is about 3% (Fig. 1).

## VI. DISCUSSION

We apply the path-integral approach using the Feynman and the generalized Luttinger-Lu method and obtain results for the limiting case of strong and weak coupling. The Feynman approach gives lower energies in the intermediate-coupling region, compared with the Luttinger-Lu approach (Fig. 1). Although the numerical results show reasonable differences, all three curves in Fig. 1 have a similar shape and the weak-coupling limit in the Feynman approach looks as it is connected with the Luttinger-Lu approach in a continuous and smooth way at  $r_s \approx 5$ . Nevertheless, in the strong-coupling limit, the two curves seem to converge to different numerical values. In the case of a metal (Fig. 2), corresponding to an intermediate value of  $r_s$ , the results differ significantly, due to the fact that none of the asymptotics in the Feynman approach is valid.

For the numerical results, we take the matrix elements of interaction  $C_k$  of the form (4), corresponding to the case of a metal. In this case, the ground-state energy for the single-particle Hamiltonian corresponds to the bottom of the conduction band.

Our results differ quantitatively from that obtained by Wigner. This discrepancy can be explained by the inappropriate dispersion law (18), which we use for this limiting case. Really, the dispersion law (18) is valid only when the random phase approximation is valid, i.e., for large electron densities. It is important to notice that Wigner's picture of the strong-coupling regime is quantitatively different from the model that is considered here, due to phase transition from uniform electron distributions, which is the background of our model, to the Wigner crystal form of distributions. So we can conclude that our results are valid in the region  $n \in (n_c, \infty)$ , where  $n_c$  is the critical density for the Wigner crystallization.

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\*Visitor from Institute of Mathematical Problem of Biology, Pushchino, Moscow region, 142292, Russia.

<sup>†</sup>Present address: National Synchrotron Research Center, Suranaree University of Technology, 111 University Avenue, Nakorn Ratchasima 30000, Thailand.

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# PHYSICAL REVIEW B

## CONDENSED MATTER AND MATERIALS PHYSICS

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### BRIEF REPORTS

*Brief Reports are accounts of completed research which, while meeting the usual Physical Review B standards of scientific quality, do not warrant regular articles. A Brief Report may be no longer than four printed pages and must be accompanied by an abstract. The same publication schedule as for regular articles is followed, and page proofs are sent to authors.*

#### Consistent definition of the effective mass of the polaron

V. Sa-yakanit and K. Tayanasanti

*Forum for Theoretical Science, Department of Physics, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand*

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The approximated density matrix of the polaron system obtained in our previous paper for deriving the Feynman effective mass  $m_F$  and the Krivoglaz-Pekar mass  $m_{KP}$  is reconsidered. It is shown that to obtain a consistent definition of the polaron effective mass one must impose the condition  $m_F = m_{KP}$ . This consistent definition is based on the fact that the wave functions derived from the density matrix corresponding to each excited state must be normalized and orthogonal. This condition leads to a consistent definition of the effective mass and a different variation principle for treating excited states. Numerical results are presented. [S0163-1829(98)05415-0]

The effective mass of the polaron problem has been studied for a long time. Many authors have used various methods to evaluate the ground-state energy and the effective mass of the polaron. Some methods are suited for a specific range of the coupling constant (see Table I of Ref. 1), but the formulation that is applicable to all coupling constants is the path-integral approach to the polaron problem by Feynman.<sup>2</sup> He showed that given a partition function, it is possible to calculate the ground-state energy as well as the effective mass of the polaron  $m_F$ . The ground-state energy was obtained by a variation calculation based on the Feynman-Jansen inequality. The variational parameters obtained are used to calculate the ground-state energy as well as the effective mass of the polaron. As pointed out by Feynman in Ref. 2, the calculation of the effective mass is not rigorous since there is no variational principle for calculating the excited state. Nevertheless, the variational parameters can be used to calculate the effective mass of the polaron. The partition function was also used by Krivoglaz and Pekar<sup>3</sup> in obtaining the different expression of the effective mass of the polaron  $m_F$  by the trace method. We shall see that this mass will appear in the full density matrix evaluated by the path-integral formulation.

Starting from the density matrix instead of the partition function, we obtain a consistent definition of the polaron effective mass. As pointed out by Sa-yakanit,<sup>4</sup> the Feynman mass and the Krivoglaz-Pekar mass are of the same density

matrix, which is obtained from the zero-temperature limit expressed in the free particle form. This limit is

$$\rho(\mathbf{R}_2 - \mathbf{R}_1; \beta \rightarrow \infty) = \left( \frac{m_{KP}}{2\pi\beta} \right)^{3/2} \times \exp \left[ -E_0\beta - \frac{m_F |\mathbf{R}_2 - \mathbf{R}_1|^2}{2\beta} \right], \quad (1)$$

where  $E_0$  is the ground-state energy of the polaron and  $\beta$  denotes the imaginary time. This expression suggests that a consistent definition of the effective mass of the polaron should be such that

$$m_F = m_{KP}. \quad (2)$$

We shall show that this condition is necessary in order for the wave function obtained from the density matrix to be normalized. The effective density matrix can also be used to obtain the excited-state wave function. The orthogonal requirement applied to each excited state leads to a different variation principle.

The starting point of our discussion is the density matrix for the polaron system

$$\rho(\mathbf{x}_2, -\mathbf{x}_1; \beta) = \int D\mathbf{x}(\tau) \exp(S), \quad (3)$$

where  $\int D[x(\tau)]$  is the path integral from  $x(0)=x_1$  and  $x(\beta)=x_1$  with

$$S = \frac{m}{2} \int_0^\beta \dot{x}(t)^2 dt - \frac{\alpha}{2^{3/2} m^{1/2}} \int_0^\beta \int_0^\beta dt ds \frac{\cosh(\beta/2 - |t-s|)/\sinh(\beta/2)}{|x(t) - x(s)|}, \quad (4)$$

where  $\alpha$  is a coupling constant between the electron and phonon and  $m$  is the electron band mass. By following Feynman, a trial action was introduced

$$S_0 = \frac{m}{2} \int_0^\beta \dot{x}(t)^2 dt - \frac{\kappa w}{8} \int_0^\beta \int_0^\beta dt ds [x(t) - x(s)]^2 \times \frac{\cosh w(\beta/2 - |t-s|)}{\sinh(w\beta/2)}. \quad (5)$$

This action corresponds to an electron coupled to a fictitious particle where  $\kappa$  and  $w$  are two parameters representing the spring constant and the frequency of a harmonic oscillator. Within the first cumulant expansion we have

$$\rho(x_2 - x_1; \beta) = \rho_0 \exp(S - S_0)_{S_0}, \quad (6)$$

where

$$\langle O \rangle_{S_0} = \frac{\int D x(t) O e^{S_0}}{\int D x(t) e^{S_0}}. \quad (7)$$

Carrying out the path integral, we have the density matrix

$$\rho(x_2 - x_1; \beta) = \rho_0 \exp \left( A + \int_0^\beta \int_0^\beta d\sigma d\tau (B + E|x_2 - x_1|^2) \right), \quad (8)$$

where

$$A = -\frac{3}{2} n \left( 1 - \frac{w^2}{v^2} \right) \left[ \frac{v\beta}{2} \coth \left( \frac{v\beta}{2} \right) - 1 \right],$$

$$B = \frac{\alpha}{2^{3/2} m^{1/2}} \int_0^\infty \frac{d^3 k}{2\pi^2 k^2} \exp \left[ i \mathbf{k} \cdot (x_2 - x_1) \mu \right. \\ \left. \times \left( \frac{\sinh \frac{v}{2} (\tau - \sigma) \cosh \frac{v}{2} [\beta - (\tau + \sigma)]}{\sinh \frac{\beta}{2}} \frac{\tau - \sigma}{M\beta} \right. \right. \\ \left. \left. - \frac{k^2}{2m v^2} F(|\tau - \sigma|, \beta) \right) \frac{\cosh w \left( \frac{v\beta}{2} - |\tau - \sigma| \right)}{\sinh \frac{v\beta}{2}} \right],$$

$$E = -\frac{C}{2} \mu^2 \left( \frac{\sinh \frac{v}{2} (\tau - \sigma) \cosh \frac{v}{2} [\beta - (\tau - \sigma)]}{\sinh \frac{v\beta}{2}} \right. \\ \left. + \frac{\tau - \sigma}{M\beta} \right)^2 \frac{\cosh w \left( \frac{\beta}{2} - (\tau - \sigma) \right)}{\sinh \frac{w\beta}{2}},$$

$$F(|\tau - \sigma|, \beta) = \mu \left( \frac{2v \sinh \frac{v}{2} (\tau - \sigma) \sinh \frac{v}{2} [\beta - (\tau - \sigma)]}{m \sinh \frac{v\beta}{2}} \right. \\ \left. + \frac{v^2 [\beta - (\tau - \sigma)] (\tau - \sigma)}{M\beta} \right),$$

and

$$\rho_0(x_2 - x_1; \beta) = \left( \frac{m}{2\pi\beta} \right)^{3/2} \left( \frac{v \sinh \frac{w\beta}{2}}{w \sinh \frac{w\beta}{2}} \right)^3 \\ \times \exp \left[ - \left( \frac{\mu v}{2} \coth \frac{v\beta}{2} + \frac{1}{2} \frac{\mu}{M\beta} \right) \right. \\ \left. \times |x_2 - x_1|^2 \right]. \quad (9)$$

Here  $v$  and  $w$  are alternative sets of variational parameters related to the previous set by the relation  $v^2 = \kappa/\mu$ ,  $M$  is the mass of the fictitious particle, and  $\mu = mM/m + M$  is the reduced mass of the system. The density matrix corresponding to the trial action was separated to distinguish it from the correction terms of the exponent. As pointed out earlier,<sup>4</sup> to obtain the effective mass from the above expressions it is necessary to go over to the center-of-mass coordinates

$$\mathbf{R} = \frac{m\mathbf{x} + M\mathbf{y}}{m + M}, \quad (10)$$

where  $\mathbf{x}$  is the electron coordinate,  $\mathbf{y}$  is the fictitious particle coordinate, and  $M$  is the fictitious particle mass. In averaging out the fictitious coordinates, the end points of  $\mathbf{y}$  were set to be equal, so we have the transformation

$$\mathbf{R}_2 - \mathbf{R}_1 = \frac{m}{m_0} (\mathbf{x}_2 - \mathbf{x}_1), \quad (11)$$

where  $m_0 = m + M$  is the total mass of the system.

For  $(x_2 - x_1) \rightarrow 0$  and  $\beta \rightarrow \infty$ , we can expand the exponent of  $B$  in Eq. (8) and keep terms up to the second order of  $\mathbf{R}_2 - \mathbf{R}_1$ . We then arrive at the density matrix of the polaron at the zero-temperature limit as in Eq. (1), with the ground-state energy and the Feynman and Krivoglaiz-Pekar effective masses defined, respectively, as

TABLE I. Our results for the two variational parameters, ground-state energies, and effective mass of the polaron (in the upper lines) for each coupling constant compared with the results calculated in Ref. 5 (in the lower lines). The values of the effective mass in parentheses were calculated from expressions (13) and (14), respectively.

| $\alpha$ | $v$   | $w$   | $m_{eff}$               | $E_0$     |
|----------|-------|-------|-------------------------|-----------|
| 1        | 2.716 | 2.48  | 1.198 19                | -1.012 93 |
|          | 3.06  | 2.83  | (1.9494,<br>1.9466)     | -1.013 02 |
| 2        | 2.841 | 2.33  | 1.485 68                | -2.054 94 |
|          | 3.237 | 2.716 | (1.473 61,<br>1.472 64) | -2.055 36 |
| 3        | 3.028 | 2.18  | 1.931 48                | -3.132 34 |
|          | 3.42  | 2.56  | (1.891 53,<br>1.888 46) | -3.133 33 |
| 4        | 3.264 | 1.99  | 2.689 36                | -4.254 47 |
|          | 3.663 | 2.368 | (2.388 75,<br>2.577 74) | -4.256 48 |
| 5        | 3.663 | 1.80  | 4.139 18                | -5.436 97 |
|          | 4.040 | 2.14  | (3.909 95,<br>3.894 17) | -5.440 14 |
| 6        | 4.396 | 1.61  | 7.452 20                | -6.707 04 |
|          | 4.667 | 1.874 | (6.870 53,<br>6.836 90) | -6.710 87 |
| 7        | 5.575 | 1.43  | 15.2030                 | -8.109 45 |
|          | 5.810 | 1.604 | (14.4544,<br>14.3908)   | -8.112 69 |
| 8        | 7.414 | 1.30  | 35.5344                 | -9.693 35 |
|          | 7.588 | 1.403 | (31.6807,<br>31.5851)   | -9.695 37 |
| 9        | 9.877 | 1.22  | 65.5548                 | -11.4846  |
|          | 9.851 | 1.283 | (62.8567,<br>62.7329)   | -11.4858  |
| 10       | 12.72 | 1.17  | 118.221                 | -13.4888  |
|          | 12.48 | 1.21  | (111.992,<br>111.849)   | -13.4904  |
| 11       | 15.34 | 1.13  | 184.296                 | -15.7094  |
|          | 15.41 | 1.162 | (183.215,<br>13.066)    | -15.7098  |
| 12       | 19.00 | 1.11  | 293.163                 | -18.1419  |
|          | 18.67 | 1.136 | (281.742,<br>281.499)   | -18.1434  |
| 13       | 22.40 | 1.09  | 422.105                 | -20.7901  |
|          | 22.17 | 1.11  | (412.442,<br>412.218)   | -20.7907  |
| 14       | 25.51 | 1.07  | 568.366                 | -23.6497  |
|          | 25.99 | 1.09  | (582.859,<br>582.681)   | -23.6513  |
| 15       | 29.62 | 1.06  | 781.014                 | -26.7234  |
|          | 30.08 | 1.077 | (797.441,<br>797.250)   | -26.7249  |
| 16       | 33.72 | 1.05  | 1031.17                 | -30.0085  |
|          | 34.46 | 1.067 | (1064.22,<br>1064.28)   | -30.0114  |

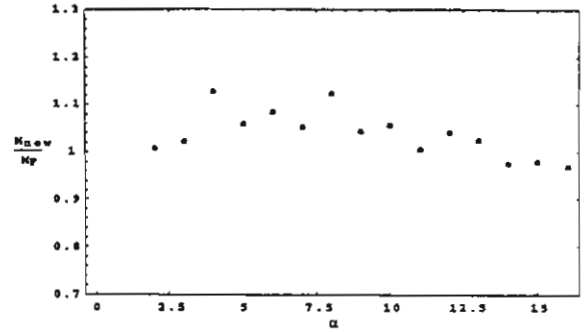


FIG. 1. Our results of the effective mass normalized to the Feynman masses  $m_F$  as a function of the coupling constant  $\alpha$ .

$$E_0 = \frac{3}{4} \frac{(v-w)^2}{v} - \frac{\alpha v}{\sqrt{\pi}} \int_0^\infty dx e^{-x} F(x)^{-1/2}, \quad (12)$$

$$m_F = 1 + \frac{\alpha}{3\sqrt{\pi}} \int_0^\infty dx v^3 x^2 e^{-x} F(x)^{-3/2}, \quad (13)$$

$$m_{KP} = \left(\frac{v}{w}\right)^2 \exp\left(\frac{w^2}{v^2} - 1 + \frac{w^2}{v^2} \frac{\alpha v^3}{\sqrt{\pi}} \int_0^\infty dx x^2 e^{-x} F(x)^{-3/2}\right), \quad (14)$$

where  $F(x) = w^2 x + v(1 - w^2/v^2)(1 - e^{-vx})$ . The two parameters must be determined by minimizing the ground-state energy and substituting it back into the expression (12) for the ground-state energy and into Eqs. (13) and (14) for the effective masses. The wave function of the polaron can be obtained from this density matrix by noticing that

$$\begin{aligned} \int_{-\infty}^{\infty} d^3k \exp\left[-\frac{2\pi^2\beta}{m_{KP}} k^2 + 2\pi i k \cdot |\mathbf{R}_2 - \mathbf{R}_1| \sqrt{\frac{m_F}{m_{KP}}}\right] \\ = \left(\frac{m_{KP}}{2\pi\beta}\right)^{3/2} \exp\left(-\frac{m_F |\mathbf{R}_2 - \mathbf{R}_1|^2}{2\beta}\right). \end{aligned} \quad (15)$$

Then

$$\begin{aligned} \rho = \int \frac{V d^3p}{(2\pi)^3} \left(\frac{m_{KP}}{m_F}\right)^{3/2} \frac{1}{V} \exp\left[i\mathbf{p} \cdot |\mathbf{R}_2 - \mathbf{R}_1| \right. \\ \left. - \left(E_0 + \frac{\mathbf{p}^2}{2m_F}\right)\beta\right]. \end{aligned} \quad (16)$$

From this expression we can obtain the unnormalized wave functions and the energies of the polaron as

$$\Psi_p(\mathbf{R}) = \frac{1}{\sqrt{V}} \sqrt{\frac{m_{KP}}{m_F}} \exp[i\mathbf{p} \cdot \mathbf{R}], \quad (17)$$

$$E_p = E_0 + \frac{\mathbf{p}^2}{2m_F}. \quad (18)$$

Because of the translational invariant, the wave functions behave like plane waves. Therefore, all wave functions become orthonormal because

$$\int d^3R \Psi_{\mathbf{p}}^*(\mathbf{R}) \Psi_{\mathbf{p}'}(\mathbf{R}) = \left( \frac{m_{KP}}{m_F} \right)^{3/2} \delta(\mathbf{p} - \mathbf{p}'). \quad (19)$$

Since all wave functions must be orthonormal, we must have  $m_F = m_{PK}$  as in our conjecture. Thus we have shown that the Feynman mass and the Krivoglaz-Pekar mass should be equal. In order to obtain the variational parameters for the effective mass or for excited states, we minimize the energy with respect to the two parameters  $v$  and  $w$  with the constraint  $m_F = m_{PK}$ . Note that any constraints on the ground-state energy will lead to a higher energy. Thus we consider this method to be a more appropriate variational principle for the effective mass. The calculated energies are presented in Table I. For comparison, we present the ground-state energies and the effective masses of Feynman calculated by Lu and Rosenfelder.<sup>5</sup> From this table it is evident that our ground-state energy is slightly higher than that of Feynman. These are not unexpected results since any constraint variational calculation will give an energy higher than the ground

state indicating the low-lying excited state. The difference in energy is quite small. In Fig. 1 we present the effective mass normalized by  $m_F$ .

In conclusion, we have shown that given the approximated density matrix proposed by Sa-yakanit,<sup>4</sup> it is possible to obtain both the ground-state energy and the effective mass. This definition of effective mass is obtained from the fact that all wave functions derived from the density matrix should be orthonormal. The variational principle used to obtain the effective mass is appropriate for the excited state as can be demonstrated by calculating the constraint ground-state energy, which is slightly higher than the ground-state energy of the polaron. Although we have no rigorous proof of this variational principle, we believe that the constraint variational principle should be the correct parameters for the excited state and therefore for the effective mass as well.

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# Bose–Einstein condensation in nonuniform media

Virulh Sa-Yakanit<sup>a</sup>, Vladimir Yarunin<sup>b</sup>, Pornther Nisamaneephong<sup>a</sup>

<sup>a</sup> *Forum for Theoretical Science, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand*

<sup>b</sup> *Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna 141980, Russian Federation*

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## Abstract

The Bogoliubov model of a nonideal gas is developed for Bose–Einstein condensation (BEC) in media with broken translational symmetry. A decrease of the transition temperature  $T_\lambda$  is found as a function of the ratio  $F_1/g_0$ , where  $g_0$  is the interaction between the atoms of the condensate and  $F_1$  is the condensate–noncondensate interaction, generated by the nonhomogeneous property of the matter. The shift of  $T_\lambda$  in porous media experimentally found by Wong et al. [Phys. Rev. Lett. 65 (1990) 2410] is applied to estimate the ratio  $F_1/g_0$ , which is found to be equal to 0.1, and may be considered as a measure of the influence of the porosity on the interaction between the atoms. © 1998 Published by Elsevier Science B.V.

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Experiments on Bose–Einstein condensation (BEC) in limited volumes (liquid  $^4\text{He}$  in porous media [1] and cold trapped atoms [2]) have been discussed recently. In both cases we deal with a non-homogeneous structure of matter, which cannot be described by a theory based on the translational invariant postulate. Therefore, the ordinary theory of BEC must be revised for nonuniform media.

With this in mind we here develop the Bogoliubov quantum-statistical model  $h_B$  of a nonideal Bose gas [3], applied recently [4–6] to BEC in  $^4\text{He}$ . We consider an additional interaction, which appears in non-homogeneous matter due to the loss of translation invariance and which is omitted ordinarily. A decrease of the BEC critical temperature is found for this case.

Let us start with [7] deducing the Hamiltonian of  $h_B$  type via the C-number shift

$$b_k^+ \rightarrow b_k^+ + \delta_{k,0} a^*, \quad b_k \rightarrow b_k + \delta_{k,0} a$$

of the annihilation and creation amplitudes of the bosons in the total Hamiltonian  $H$  of the nonideal Bose gas. This shift separates the particles of the Bose condensate with zero momentum  $k = 0$  (treated as classical particles) from the noncondensate bosons with momentum  $k \neq 0$  (treated as quantum particles),

$$H \rightarrow h = h_B + h_1, \quad (1)$$

$$h_B = g_0 \frac{|a|^4}{2V} + \sum_{k \neq 0} \left( \Omega_k b_k^+ b_k + \frac{g_k}{2V} (b_k^+ b_{-k}^+ a^2 + b_k b_{-k} a^2 + 2b_k^+ b_k |a|^2) + \frac{g_0}{V} b_k^+ b_k |a|^2 \right),$$

$$\Omega_k = \frac{k^2}{2m}, \quad [b_k, b_{k'}^+] = \delta_{kk'},$$

$$h_1 = \sum_{k \neq 0} \frac{g_{k,0}}{V} (b_k^+ a^* a^2 + b_k a a^{*2}),$$

$$g_0 = \langle 0, 0 | g | 0, 0 \rangle,$$

$$g_k = \langle k, 0 | g | k, 0 \rangle = \langle k, -k | g | 0, 0 \rangle,$$

$$g_{k,0} = \langle k, 0 | g | 0, 0 \rangle.$$

Here  $g_0, g_k$ , and  $g_{0,k}$  are the matrix elements of the interaction potential  $g(x, y)$ , which depends on the three-dimensional space points  $x, y$  separately, but not on the combination  $(x - y)$ , as in the space-uniform system. This model is used here – contrary to the random external field approach [8] – in order to empirically describe the deformation of atomic polarizations near the walls of the pores.

The deduced approximation (1) for the total Hamiltonian  $H$  neglects the nonuniform effects of the interaction between the particles within each of the subsystems of condensate and noncondensate bosons but describes these effects for the inter-subsystem interaction. Therefore, only the terms responsible for the pair correlations between the noncondensate bosons are considered in the Bogoliubov Hamiltonian  $H_B$ ; it is translation invariant. The term  $h_1$  breaks the translation symmetry, but conserves the “quasi-classical” number of particles,

$$\{h_1, |a|^2\} + i \left[ h_1, \sum_{k \neq 0} b_k^+ b_k \right] = 0,$$

$$\{h_1, \} = i \left( \frac{\partial h_1}{\partial a} \frac{\partial}{\partial a^*} - \frac{\partial h_1}{\partial a^*} \frac{\partial}{\partial a} \right).$$

The same property was found earlier [5,6] for the Bogoliubov interaction  $H_B$  and so the “quasi-classical” integral of motion  $n$ ,

$$\frac{dn}{dt} = \frac{d}{dt} \left( |a|^2 + \sum_{k \neq 0} b_k^+ b_k \right) = 0, \quad (2)$$

exists for the system (1). Following Refs. [5,6] we consider the partition function with constraint, due to the  $n$ -conservation law (2) for  $N$  bosons in Eq. (1),

$$Q = \text{Sp} (e^{-\beta H} \delta_{N,n}),$$

as an integral over the variables  $a, a^*$  and a functional integral over the trajectories  $b_k, b_k^*$  with the periodical boundary conditions

$$Q = \int d^2 a \prod_{k \neq 0} \int Db_k^* Db_k \int_{-\pi}^{\pi} dy \exp \left( i y (|a|^2 - N) - \beta \frac{g_0}{2V} |a|^4 + \Phi \right). \quad (3)$$

Here the Fourier decomposition of the  $\delta$ -function with the spectral parameter  $\nu = i y \beta^{-1}$  is introduced and the functional  $\Phi$  looks like

$$\begin{aligned} \Phi &= \sum_{k \neq 0} \Phi_k \\ &= \int_0^\beta dt \sum_{k \neq 0} \left[ (b_k^*, b_{-k}) P_k \begin{pmatrix} b_k \\ b_{-k}^* \end{pmatrix} \right. \\ &\quad \left. + (b_k^*, b_{-k}) f_k + f_k^* \begin{pmatrix} b_k \\ b_{-k}^* \end{pmatrix} \right], \\ P_k &= \begin{pmatrix} -d/dt - \omega_k + \nu & -\gamma_k \\ -\gamma_k^* & d/dt - \omega_k + \nu \end{pmatrix}, \end{aligned}$$

$$\omega_k = \Omega_k + (g_0 + g_k) \rho, \quad \rho = \frac{|a|^2}{V},$$

$$\gamma_k = \frac{g_k}{2V} a^2,$$

$$f_k^* = (a a^*) \rho \frac{g_{0,k}}{2}, \quad f_k = \left( \frac{a}{a^*} \right) \rho \frac{g_{k,0}}{2},$$

where  $\rho$  is the Bose condensate density. The functional integral over the trajectories  $b_k, b_k^*$  in  $Q$  may be calculated via the formula

$$\begin{aligned} \int Db_k^* Db_k \exp(\Phi_k) &= \frac{\exp(A_k)}{\text{Det}(-P_k)}, \\ A_k &= \int_0^\beta f_k^* (-P_k)^{-1} f_k dt. \end{aligned} \quad (4)$$

In the following we use the result of the calculation of  $\text{Det}(-P_k)$ , given in Refs. [5,6] (see the details in Ref. [9]),

$$[\text{Det}(-P_k)]^{-1} = \frac{\exp(\omega_k - \nu) \beta / 2}{4 \sinh^2(\beta E_k / 4)},$$

and notice that

$$A_k = -\beta (f_k^* M^{-1} m f_k), \quad m = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}.$$

$$M = \begin{pmatrix} \omega_k - \nu & \gamma_k \\ -\gamma_k^* & -\omega_k + \nu \end{pmatrix},$$

as far as the vectors  $f_k$  are constants. The spectrum  $E_k$  of the over-condensate excitations,

$$E_k = [(\Omega_k + \rho g_0 - \nu)^2 + 2\rho g_k(\Omega_k + \rho g_0 - \nu)]^{1/2},$$

depends on the condensate density  $\rho$  and the constraint parameter  $\nu$  and coincides with the one obtained in homogeneous ( $h_1 = 0$ ) media [5,6,9]. The absence of translational invariance, a consequence of the term  $h_1$ , leads to the term  $A_k = 0$  in formula (4). A straightforward calculation of the scalar product in the term  $A_k$  leads to the expression

$$A_k = \frac{\beta V \rho^2}{4} |g_{k,0}|^2 \frac{2a^* a(\omega_k - \nu) - \gamma_k a^{*2} - \gamma_k^* a^2}{(\omega_k - \nu)^2 - |\gamma_k|^2}.$$

Taking into account the definition of  $\gamma_k$  and the exact relation  $(\omega_k - \nu)^2 = E_k^2 + 3|\gamma_k|^2$ , we introduce the approximation of a small condensate density  $\rho$  in  $A_k$ ,

$$A_k \simeq \frac{\beta V \rho^3}{2} |g_{k,0}|^2 \frac{\omega_k - \nu}{E_k^2} \simeq \frac{\beta V}{2} |g_{k,0}|^2 \frac{\rho^3}{E_k}. \quad (5)$$

This approximation means that only the lowest degree  $\rho^3$  is considered in  $A_k$  and this is adequate for the temperature not close to zero, when the condensate density is not large. Now with the use of formulae (4) and (5) the effective action  $S_{\text{ef}}$  of the condensate bosons is introduced in the partition function (3) of the system (1),

$$Q = \int d\rho d\nu \exp(S_{\text{ef}}), \quad S_{\text{ef}} = S_B + S_1,$$

$$S_B = -\beta V (g_0 \rho^2 / 2 - \nu \rho + \nu R) \\ + cV \int k^2 [(\omega_k - \nu)\beta/2 - 2 \ln \sinh(\beta E_k/4)] dk,$$

$$S_1 = \beta V \rho^3 \frac{c}{2} \int k^2 \frac{|g_{k,0}|^2}{E_k} dk, \quad c^{-1} = 2\pi^2 h^3,$$

$$R = \frac{N}{V}.$$

The term  $S_1$  is responsible for the broken translational symmetry and the term  $S_B$  is just the term  $S_{\text{ef}}$  of Refs. [5,6]. We would like to recall once more that only the processes of condensate–noncondensate scattering induced by the loss of the translational invariance are considered in Eq. (1), while the modification

of  $S_B$  for the same reason is neglected. The matrix elements  $g_0, g_k$  and  $g_{k,0}$  in formulae (1) and (5) in fact depend on the details of the interaction between the bosons in the presence of porous media in  $^4\text{He}$ , but in the present Letter they are considered as empirical parameters. Now the variational equations  $\delta S_{\text{ef}} = 0$  in the limit  $N, V \rightarrow \infty$  with respect to the variables  $\rho$  and  $\nu$  must be considered, and we obtain these equations in the form

$$r + \rho = R, \quad \nu - \rho g_0 - 2r g_0 + \rho F_0 + \frac{1}{R} \rho^2 F_1 = 0, \quad (6)$$

where  $r$  is the density of the noncondensate bosons. Eqs. (6) (with  $F_1 = 0$  in uniform media) were obtained in Refs. [6,9] and the second equation of (6) with the additional assumption of a small condensate density,  $\rho \ll R$ ,  $F_0 = 0$  was obtained in Ref. [10]. In view of the contribution of  $\partial E_k / \partial \rho$ ,  $\partial E_k / \partial \nu$  for  $S_1$  in Eq. (6) being of the next order in  $\rho$  compared to the one considered above in  $A_k$ , we use the functionals  $r$ ,  $F_0$ , and  $F_1$  in the form

$$r = \frac{c}{2} \int k^2 [\coth(\beta E_k/4) - 1] dk,$$

$$F_0 = \frac{c}{2} \int k^2 \coth(\beta E_k/4) \frac{g_k^2}{E_k} dk,$$

$$F_1 = \frac{3c}{2} \int k^2 \frac{|g_{k,0}|^2}{E_k} dk, \quad F_1 < 3F_0.$$

The no-gap condition for the spectrum  $E_k$  leads to the values  $\nu_1 = g_0 \rho$ ,  $\nu_2 = 3g_0 \rho$  for the “non-trivial” and “trivial” solutions of Eq. (6), respectively. The linearization  $F(\rho) \rightarrow F_0(\rho_0)$  with the condensate density  $\rho_0$  of the ideal Bose gas is assumed here as in Refs. [4–6]. Then, being interested only in the superfluid state of  $^4\text{He}$  we put  $\nu_1 = g_0 \rho$  in Eq. (6) and get

$$2g_0(\rho - R) + \rho F_0 + \frac{1}{R} \rho^2 F_1 = 0. \quad (7)$$

Now we would like to compare the solution  $\rho_1$  of Eq. (7) with the solution  $\rho$  in the case of uniform media [5,6],

$$F_1 = 0, \quad 2g_0(\rho - R) + \rho F_0 = 0,$$

$$\rho = \frac{R}{1+x}, \quad x = \frac{F_0}{2g_0}.$$

To simplify the formulae we consider the weak non-homogeneity factor with inequality  $|g_{k,0}|^2 \ll g_k^2$  (that

is  $F_1 \ll F_0$ ) and obtain the solution  $\rho_1$  of Eq. (7) in the form

$$\rho_1 \simeq \rho - \frac{F_1}{R(2g_0 + F_0)} \rho^2.$$

The value  $x$  was estimated as  $x \sim 5$  in Ref. [5] for temperatures not close to zero and to the critical temperature. Therefore, the following relations are deduced for this temperature region,

$$\begin{aligned} \rho_1 &\simeq \frac{R}{x} \left( 1 - \frac{F_1}{xF_0} \right), \quad \frac{\rho_1}{\rho} \simeq 1 - \alpha, \\ \alpha &= \frac{2g_0 F_1}{F_0^2}. \end{aligned} \quad (8)$$

The ratio  $F_1/g_0$  is a measure of the pores' influence on the Bose condensate. The interaction  $F_0$  between the noncondensate bosons exceeds, as we have seen above, the interaction  $g_0$  between the bosons of the condensate (we assume these to be the same in uniform and nonuniform media). The value of  $F_0$  also exceeds the condensate–noncondensate interaction  $F_1$ , due to the loss of translational symmetry of the system (1). In order to make some estimates let  $\coth(\beta E_k/4) \sim 4/\beta E_k$  in the terms  $F_0, F_1$  of Eq. (6) (the temperature is not close to 0 K) obtaining the formulae for the noncondensate densities  $r$  and  $r_1$  in the form

$$r = TA - B, \quad r_1 = TA_1 - B,$$

$$R = r|_{T_\lambda} = AT_\lambda - B = r_1|_{T_{\lambda_1}} = A_1 T_{\lambda_1} - B.$$

Here  $A, A_1$  and  $B$  are some integrals over the  $k$  variable. We do not need to calculate them, because they are excluded in the ratio of densities

$$\frac{\rho_1}{\rho} = \frac{R - r_1}{R - r} = \frac{T_\lambda T_{\lambda_1} - T}{T_{\lambda_1} T_\lambda - T}, \quad T_\lambda = T_\lambda|_{h_1=0},$$

$$T_{\lambda_1} = T_\lambda|_{h_1 \neq 0}. \quad (9)$$

The substitution

$$T = z \frac{T_\lambda T_{\lambda_1}}{T_\lambda + T_{\lambda_1}}, \quad 0 < z < 1,$$

into Eq. (9) leads to the equation

$$1 > \frac{\rho_1}{\rho} = 1 - \frac{z(T_\lambda - T_{\lambda_1})}{T_\lambda + T_{\lambda_1}(1 - z)} \sim \frac{T_{\lambda_1}}{T_\lambda}, \quad z \sim 1. \quad (10)$$

The last ratio for  $z \sim 1$  corresponds to the temperature region between zero and the critical temperature.

The result (10) confirms the main tendency noticed in the experiment [1]: the decrease of the superfluid  $T_\lambda$  in nonuniform (porous) media. This tendency means that BEC is the effect merely of Bose statistics and it is smeared out by the interaction between the bosons. In fact, this interaction in uniform media decreases the critical temperature of the ideal Bose gas from  $\sim 3.2$  K to  $\sim 2.17$  K, and the additional perturbation, supplied by the nonhomogeneity of the sample, decreases this temperature by the factor  $\alpha \ll 1$  in formula (8) of the present Letter. Taking into account the experimental [1] ratio  $T_\lambda|_{h_1 \neq 0} (T_\lambda|_{h=0})^{-1} = 2.168 \times (2.172)^{-1} \simeq 0.998$ , we may represent  $\alpha$  as

$$\alpha \simeq 0.002 \simeq \left( \frac{2g_0}{F_0} \right)^2 \frac{F_1}{2g_0}$$

and get the estimate  $F_1/g_0 \sim 0.1$ . As we treat  $F_1$  as the deformation factor for atoms near the walls of the pores, we may consider this factor as the ratio of the number of bosons with the “hard core” type interaction near the walls to the number of bosons with the “van der Waals” type interaction in the middle part of the pores. These values may give a key to the structure of the matrix elements in the model (1) and lead to the development of the microscopic theory of BEC in porous media.

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# Path integral and variation method in the band tail problem

V. Sa-yakanit

*Forum for Theoretical Science, Department of Physics, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand*

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## Abstract

A one-dimensional random system represented by a tridiagonal random matrix with diagonal elements distributed independently in Gaussian fashion as proposed by Bulatov and Birman [Phys. Rev. B 54 (1996) 16 305] for the calculation of the density of states in the band tails is formulated in terms of Feynman path integrals. It is shown that in the asymptotic limits both the prefactor and the exponent give the correct energy dependence for the density of states. A precise comparison of the random matrix theory and the path integral approach is given. © 1998 Elsevier Science B.V.

The one-dimensional white noise model is a simple example of a disordered system for which an exact expression of the density of states exists. This was first pointed out by Frish and Lloyd [1] and has subsequently been studied in detail by Halperin [2] using the Green function method, by Zittartz and Langer [3] using the functional integration method, by Sa-yakanit [4] using the Feynman path integral method, by Edwards and Anderson [5] using the replica method and by Efetov [6] using the supersymmetry method. All of these methods lead to the same asymptotic form of the density of states (DOS),

$$\rho_{\text{as}}(E) = \frac{A(E)}{2\xi} \exp\left(-\frac{B(E)}{2\xi}\right), \quad (1)$$

where  $A(E)$  is the prefactor function and  $B(E)$  is a function of the exponent. Here  $\xi$  is the fluctuation parameter, denoting the strength of the randomness of the system. The explicit forms of  $A(E)$  and  $B(E)$  are

$$A(E) = \alpha(-E), \quad (2)$$

$$B(E) = \beta(-E)^{3/2}, \quad (3)$$

where  $\alpha$  and  $\beta$  are constants and  $E \ll 0$ . The exact values obtained from Frish and Lloyd [1] are

$$\alpha = \frac{8}{\pi}, \quad \beta = \frac{8\sqrt{2}}{3} \frac{\hbar}{\sqrt{m}}. \quad (4)$$

In Ref. [7], Bulatov and Birman showed that this problem can be formulated and solved by using ideas from random matrix theory (RMT). They considered a simple 1D chain with diagonal disorder and showed that RMT together with a recursion method [8,9] could reproduce impurity band tails. They considered the simplest model with the hopping Hamiltonian

$$H = \sum_i \epsilon_i |a_i\rangle\langle a_i| + V|a_i\rangle\langle a_{i+1}| + V|a_i\rangle\langle a_{i-1}|, \quad (5)$$

where the diagonal elements  $\epsilon_i$  are disordered and represent the fluctuations of the potential energy at given sites. The constant  $V$  equals the band width and can be expressed in terms of the effective mass and the size of the unit cell  $b$  by

$$V = \frac{1}{2m^*b^2}. \quad (6)$$

Furthermore, they obtained an analytic form of the DOS in their whole range of energies, both in the band tail and in the high energy region. Regarding the band tail region, they obtained the correct asymptotic behaviour in the exponent with different values of  $\beta$  from the exact value given in Eq. (4). They pointed out that the complicated numerical factors  $\alpha$  and  $\beta$  are consequences of a finite correlation radius of the discrete model.

In this Letter, we show that the continuous limit of this discrete model, reformulated in terms of the Feynman path integrals, as was done in Ref. [4], is more convenient. By employing this method we can represent the system in terms of the time dependent Schrödinger equation in the tight binding representation

$$i\hbar \frac{\partial a_i(t)}{\partial t} = \epsilon_i a_i(t) + \sum_{j \neq i} a_j(t) V_{ij}. \quad (7)$$

For the one-dimensional system with nearest neighbour interaction, Eq. (7) reduces to

$$i\hbar \frac{\partial a_i(t)}{\partial t} = \epsilon_i a_i(t) + V a_{i+1}(t) + V a_{i-1}(t). \quad (8)$$

Assuming that the function  $a_{i+1}$  can be expanded about the function  $a_i$  at site  $i$  we see that, up to the second order,

$$a_{i+1}(t) = a_i(t) + b \nabla_i a_i(t) + \frac{b^2}{2} \nabla_i^2 a_i(t), \quad (9)$$

and

$$a_{i-1}(t) = a_i(t) - b \nabla_i a_i(t) + \frac{b^2}{2} \nabla_i^2 a_i(t), \quad (10)$$

where  $b$  is the lattice constant of the system. To go over to the continuum limit, we assume that  $b^2 \ll 0$ ; then  $b^2 V$  becomes constant. In this limit, Eq. (8) becomes

$$i\hbar \frac{\partial a_i(r, t)}{\partial t} = [\epsilon(r) + 2V] a(r, t) - \frac{\hbar^2}{2m} \nabla^2 a(r, t), \quad (11)$$

where  $b^2 V = -\hbar^2/2m$  is identified. Note that the new definition of  $V$  has a sign opposite to the one given in Eq. (6). For  $\epsilon = \text{const}$ , Eq. (11) is simply the free particle with shifted energy  $\epsilon + 2V$ . In the energy and momentum representation

$$a(p, E) = \int e^{-(t/\hbar)(Et + pr)} a(r, t) dt dr, \quad (12)$$

we obtain the eigenvalue

$$E = \frac{p^2}{2m} + \epsilon + 2V, \quad (13)$$

which gives the DOS in one dimension as

$$\rho(E) \sim \frac{1}{\sqrt{E - \epsilon - 2V}}. \quad (14)$$

We now introduce randomness into the system. We study the case where  $\epsilon(r)$  is distributed in a Gaussian random fashion with zero mean  $\langle \epsilon \rangle = 0$  and finite correlation length  $L$ . Then the correlation function becomes

$$\langle \epsilon(r) \epsilon(r') \rangle = W(r - r') = \xi_L e^{-|r - r'|^2/L^2}. \quad (15)$$

At this stage, it is better to keep the correlation length  $L$  as a finite quantity and consider the white noise limit at the end. In order to carry out the average, we rewrite Eq. (11) in the path integral representation

$$G(r, r', t) = \int \mathcal{D}[r(\tau)] \times \exp \left( \frac{i}{\hbar} \int_0^t \left[ \frac{1}{2} m \dot{r}^2(\tau) - \epsilon(r(\tau)) + 2V \right] d\tau \right). \quad (16)$$

The average propagator  $K(r - r'; t) = \langle G(r, r'; t) \rangle$  can then be written in the form

$$K(r - r', t) = \int \mathcal{D}[r(\tau)] \times \exp \left[ \frac{i}{\hbar} \left( \int_0^t \left[ \frac{1}{2} m \dot{r}^2(\tau) - 2V \right] d\tau + \int \int W(r(\tau) - r(\sigma)) d\tau d\sigma \right) \right] = \int \mathcal{D}[r(\tau)] e^{(i/\hbar)S}. \quad (17)$$

$K(r - r'; t)$  is approximated by the first cumulant

$$K(r - r'; t) \approx K_0 e^{(S - S_0)/S_0}, \quad (18)$$

where

$$S_0 = \int_0^t \frac{m}{2} \left( \dot{r}^2(\sigma) - \int_0^t \frac{\omega^2}{2t} |r(\tau) - r(\sigma)|^2 d\tau \right) d\sigma, \quad (19)$$

and where  $\omega$  is a variational parameter to be determined. The DOS can be obtained by taking the trace of Eq. (18), then

$$\begin{aligned}\rho(E) &= \text{Re} \int_0^\infty \text{Tr} K_1(r-r'; t) e^{(i/\hbar)Et} dt \\ &= \frac{1}{2\pi\hbar} \int_{-\infty}^\infty dt \left( \frac{m}{2\pi\hbar it} \right)^{1/2} \left( \frac{\omega t}{2 \sin(\omega t/2)} \right) \\ &\quad \times \exp \left[ \frac{i}{\hbar} (E - 2V)t + \frac{1}{2} \left( \frac{\omega t}{2} \cot \frac{\omega t}{2} - 1 \right) \right. \\ &\quad \left. - \frac{1}{2\hbar^2} \xi_L \left( \frac{L^2}{4} \right)^{1/2} t \int_0^t dx j(x, \omega; t)^{-1/2} \right], \quad (20)\end{aligned}$$

where

$$\begin{aligned}j(x, \omega; t) &= \left( \frac{L^2}{4} + \frac{i\hbar}{m\omega} \right. \\ &\quad \left. \times \frac{\sin(m\omega/2) \sin[\omega(t-x)/2]}{\sin(\omega t/2)} \right). \quad (21)\end{aligned}$$

To compute the ground state contribution, we let  $t \rightarrow \infty$  and obtain

$$\begin{aligned}\rho(E) &= \frac{1}{2\pi\hbar} \int_{-\infty}^\infty dt \left( \frac{m\omega^2}{2\pi i\hbar} \right)^{1/2} (it)^{1/2} \\ &\quad \times \exp \left[ \frac{i}{\hbar} \left( -\frac{E_\omega}{4} + (E - 2V) \right) t \right. \\ &\quad \left. - \frac{1}{2\hbar^2} \xi_L \left( \frac{L^2}{4} \right)^{1/2} \frac{t^2}{(L^2/4 + \hbar/2m\omega)^{1/2}} \right], \quad (22)\end{aligned}$$

where  $E_\omega = \hbar\omega$ . In the white noise limit as  $L \rightarrow 0$ , the DOS becomes

$$\begin{aligned}\rho(E) &= \frac{1}{2\pi\hbar} \left( \frac{m\omega^2}{2\pi\hbar} \right)^{1/2} \frac{1}{2^{1/4}} \sqrt{\pi} \beta^{-3/2} \\ &\quad \times \exp \left( -\frac{q^2}{4\beta^2} \right) \left( \frac{q}{\beta\sqrt{2}} \right)^{1/2}, \quad (23)\end{aligned}$$

where

$$\begin{aligned}q &= \frac{E_\omega/4 - E - 2V}{\hbar}, \\ \beta^2 &= \frac{\xi_L}{2\hbar^2} \left( \frac{mE_\omega}{2\pi\hbar^2} \right)^{1/2}. \quad (24)\end{aligned}$$

Taking the asymptotic limit as  $\xi_L \rightarrow 0$ , we maximize the exponent

$$\frac{d}{d\omega} \frac{q^2}{2\beta^2} = 0. \quad (25)$$

This leads to  $E_\omega = -\frac{4}{3}(E - 2V)$ . Then we obtain that the final result for  $E \ll 0$  is

$$\begin{aligned}\rho(E) &= \sqrt{\frac{2\pi}{6}} \frac{4 - E + 2V}{\pi \xi_L} \\ &\quad \times \exp \left[ -\left( \frac{\pi}{3} \right)^{1/2} \frac{4\sqrt{2}}{3} \frac{\hbar}{\sqrt{m}} \frac{(-E + 2V)^{3/2}}{\xi_L} \right]. \quad (26)\end{aligned}$$

We note that for positive energy,  $E \gg 0$ , Eq. (20) gives the free particle.

We can compare this result with that obtained by an exact calculation [1]. We find the agreement between our results and the exact result to be very good. The powers of  $E$  in the exponent and in front of the exponential are correct. The numerical factor in the exponent differs from the exact value by a factor of  $(\pi/3)^{3/2} = 1.0233$ . The numerical factor in front of the exponent is too small by a factor  $6/2\pi = 2.393$ .

We can also compare our results with that of Bulatov and Birman (BB) [7]. Their result can be rewritten in the present expression as

$$\begin{aligned}\rho(E) &\sim \frac{1}{\sqrt{E/2 + V}} \\ &\quad \times \exp \left[ -\frac{1}{2\sigma^2} \frac{5}{4} \sqrt{V} \left( -\frac{E}{2} - V \right)^{3/2} \right], \quad E \ll 0,\end{aligned}$$

and in our notation,

$$\begin{aligned}\rho(E) &\sim \frac{1}{\sqrt{E/2 - V}} \exp \left( -\frac{45\sqrt{2}}{256} \beta \frac{8\sqrt{2}}{3} \frac{\hbar}{\sqrt{m}} \right. \\ &\quad \left. \times \frac{(-E - 2V)^{5/2}}{\xi_L} \right), \quad E \ll 0, \quad (27)\end{aligned}$$

where  $\xi_L \sim \sigma b$ . Note that our  $\xi_L$  and  $\sigma$  differ by a factor  $b$ .

In conclusion, we have shown that the discrete band tail model in one-dimensional white Gaussian noise proposed by BB using RMT can be reformulated using a Feynman path integral. We showed that the Feynman path integral gives the correct energy dependent

behaviour both in the prefactor and the exponent as compared with the exact result of Ref. [1], while BB give only the correct behaviour in the exponent. The discrepancy in the exponent in our case is a factor of  $(\pi/3)^{1/2}$ , while that of Ref. [7] is a factor of  $(45/256) \times 2^{1/2}$ . As discussed by BB, their result was obtained by a first order iteration and certainly is not exact, but it gives the correct power energy dependence.

It is interesting to point out that the path integral method using a single harmonic as well as a trial action will not enable us to obtain the exact result for the white Gaussian noise fluctuation. This is because the white noise potential has a bound state at  $-\infty$ . The approach of Halperin and Lax [10], Zittartz and Langer [3] and Lifshitz [11], called the “optimal fluctuation method”, can obtain the exact result because the variation equation is a non-linear integro-differential equation, and in one dimension there exists an exact soliton solution. A more rigorous approach to this problem was given by Efetov [6] using the supersymmetry method. His method is not as general as the replica method and only applicable to the description of non-interacting particles, having random potentials. It is based on the use of functional integration over both commuting and anti-commuting variables. This makes it possible to represent physical quantities in a form which enables their method to average over impurities at the beginning of the calculation. The averaging over the impurities has been done

also in our calculation before performing the path integral. This method was applied to one-dimensional Gaussian white noise and equations were obtained similar to those of Halperin and Lax [10] and Frish and Lloyd [1]. The path integral approach has the advantage of easy generalization to any dimensions, with different correlation lengths [12] and different systems like heavily doped semi-conductor ones [4], and to the quantum Hall problem [3]. An improvement of the calculation can be realised by introducing a two parameter trial action or by considering higher cumulant expansions.

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## PATH INTEGRAL CALCULATIONS OF PARTICLE SELF-ENERGY AND EFFECTIVE MASS IN COULOMB SYSTEMS

V. SA-YAKANIT, V. D. LAKHNO\*, and KLAUS HAB

*Forum for Theoretical Science, Faculty of Science,  
Chulalongkorn University, Bangkok, 10330, Thailand*

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The generalized path integral approach is applied to calculate the ground state energy and the effective mass of an electron-plasmon interacting system for a wide range of densities. It is shown that in the self-consistent approximation an abrupt transition between the weak coupling and the strong coupling region of interaction exists. The transition occurs at low electron densities according to a value of 418 for  $r_s$ , when Wigner crystallization is possible. For densities of real metals, the electron bandwidth is calculated and a comparison with experimental results is given.

### 1. Introduction

The electron-plasmon coupling in solids has been discussed by many authors since the pioneering work by Bohm and Pines.<sup>1</sup> Lundquist<sup>2</sup> showed that the interaction of an individual electron with plasmons in the random phase approximation (RPA) can be described in terms of the Fröhlich-type interaction Hamiltonian in analogy with the polaron problem.<sup>3</sup> This form of the electron-plasmon interaction in metals may be called the "plasmaron coupling".<sup>2,4</sup>

Recently the quantum theory of self-localization has been developed for electrons in semiconductor plasma.<sup>5</sup> In the case of a  $p$ -type semiconductor the electron in the conduction band has been considered as a probe particle, the same like a hole in the valence band in the case of an  $n$ -type semiconductor.

The electron surrounded by a cloud of screening holes in the conduction band of a  $p$ -type semiconductor forms a zero charged quasiparticle which was called a continuum exciton.<sup>6</sup> In Refs. 5 and 6 only the limiting cases of weak and strong electron-plasmon interaction were considered.

The main purpose of this paper is to develop a theory and to calculate the self-energy and the effective mass of plasmarons for intermediate values of interaction.

\*On leave from Institute of Mathematical Problems of Biology Pushchino, Moscow Region, 142292, Russia.

In this work we apply the generalized path integral approach to describe the particle coupled with plasmons. For metals the path integral method was first developed in Ref. 7 and for semiconductors in Ref. 8. As it was first demonstrated by Feynman,<sup>3</sup> the path integral approach gives the best results for the intermediate coupling interaction in the case of electron-plasmon coupling. This case is usually realized in real systems mentioned above, where electron-plasmon interaction gives the main input at intermediate values of the coupling constant.

In order to calculate the self-energy and effective mass at intermediate values of the coupling constant, we apply the generalized path integral method.<sup>9</sup> The generalization is introduced by a trial model, where a particle interacts with a second particle by means of arbitrary potential  $V(\underline{r}, \underline{r}')$ , which is used for variational calculations.

In Sec. 2 we reproduce the main ideas of the generalized path integral approach and obtain the expression for the ground state energy in the case of electron-plasmon interaction. In Sec. 3 we represent the numerical results for the ground state energy in a self-consistent approximation. In Sec. 4 the expression for the effective mass due to the dressing of the electron by a cloud of plasmons is described. The results of the numerical calculations of the effective mass are presented in Sec. 5. In Sec. 6 the obtained results are applied to the calculation of the electron bandwidth in metals and are compared with experimental data.

## 2. Self-Energy

The main problem of the calculation of properties of quantum mechanical systems by the method of path integrals is connected with the problem of calculating the evolution propagator

$$\langle \underline{r}'', t'' | \underline{r}', t' \rangle = \int D\underline{r}(t) e^{i \frac{\tilde{S}}{\hbar}}. \quad (1)$$

In case of electron-plasmon interaction the Lagrangian  $L$  is equal to<sup>7,8</sup>:

$$L = \frac{m}{2} \dot{r}^2(t) + \sum_k L_k, \quad (2)$$

$$L_k = \frac{1}{2} \dot{q}_k^2 - \frac{\omega_k^2}{2} q_k^2 + \sqrt{2\omega_k} c_k e^{ikr} q_k,$$

where  $\underline{r}(t)$  and  $q_k$  are the electron and plasmon coordinates,  $\underline{k}$  is the wavevector,  $m$  is the electron effective mass and

$$c_k = i \frac{e}{k} \sqrt{\frac{4\pi\hbar}{\Omega(\partial\varepsilon(\omega, k)/\partial\omega)_{\omega=\omega_p}}}, \quad (3)$$

where  $\Omega$  is the volume of the system. The dielectric function  $\varepsilon(\omega, k)$  is given by the relation:

$$\varepsilon(\omega, k) = \frac{\omega_k^2 - \omega^2}{\omega_k^2 - \omega_p^2 - \omega^2} \quad (4)$$

where  $\omega_p = \sqrt{4\pi ne^2/m}$  is the plasma frequency for long wave plasmons and electron density  $n$ . The plasmon dispersion law is taken as:

$$\omega_k^2 = \omega_p^2 + \frac{1}{3} \left( \frac{\hbar k_F}{m} \right)^2 k^2 + \left( \frac{\hbar k^2}{2m} \right)^2. \quad (5)$$

In (5)  $\hbar k_F$  is the Fermi momentum, and the coefficient in front of the  $k^2$  term is a factor of 5/9 smaller than the RPA coefficient. It is chosen in order to give the correct Thomas-Fermi potential in the static long wave limit. It was pointed out by Lundquist that the  $k^2$  term for real metals is less important than the  $k^4$  term. The form of the dielectric function in (4) is chosen in order to produce the following sum rules:

$$\int_0^\infty d\omega \omega \text{Im} \left( \frac{1}{\varepsilon(k, \omega + i\delta)} \right) = -\frac{\pi}{2} \omega_p^2, \quad (6)$$

$$\int_0^\infty d\omega \omega \text{Im} (\varepsilon(k, \omega + i\delta)) = \frac{\pi}{2} \omega_p^2. \quad (7)$$

According to (1) and (2) the ground state energy of the considered system is equal to:

$$\begin{aligned} E_0 &= - \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \ln \int D\underline{r}(t) e^{-S(\underline{r})}, \\ S(\underline{r}) &= \frac{m}{2} \int_0^\beta d\tau \dot{\underline{r}}^2(\tau) + V(\underline{r}), \\ V(\underline{r}) &= -2 \sum_k |c_k|^2 \int_0^\beta d\tau \int_0^\tau d\sigma e^{-(\tau-\sigma)\omega_k + i\mathbf{k}(\underline{r}(\tau) - \underline{r}(\sigma))}. \end{aligned} \quad (8)$$

In (8) and the following equations we set  $\hbar = 1$ . Following Ref. 8 we can take the probe action  $S_0(\underline{r}, \underline{r}')$  of the form:

$$\begin{aligned} S_0(\underline{r}, \underline{r}') &= \frac{m}{2} \int_0^\beta d\tau \dot{\underline{r}}^2(\tau) + \frac{m'}{2} \int_0^\beta d\tau \dot{\underline{r}}'^2(\tau) + V_0(\underline{r}, \underline{r}'), \\ V_0(\underline{r}, \underline{r}') &= \int_0^\beta d\tau U[\underline{r}(\tau) - \underline{r}'(\tau)], \end{aligned} \quad (9)$$

where  $m'$  is the mass of a probe particle and  $U$  is the probe potential.

The upper limit of the ground state energy (8) can be obtained by Jensen's inequality:

$$E_0 \leq \varepsilon_0 + \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \langle V - V_0 \rangle_{S_0}, \quad (10)$$

where

$$\varepsilon_0 = - \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \ln \int \int_{\underline{r}(0)=\underline{r}(\beta), \underline{r}'(0)=\underline{r}'(\beta)} D(\underline{r}) D(\underline{r}') e^{-S_0(\underline{r}, \underline{r}')}. \quad (11)$$

According to the generalized path integral method:

$$\varepsilon_0 - \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \langle V_0 \rangle_{S_0} = -\frac{1}{2\mu} \int d^3x U_0^*(x) \Delta U_0(x) \quad (12)$$

where  $U_0(x)$  is the wave function of the ground state for the Hamiltonian

$$H_0 = -\frac{1}{2\mu} \Delta + V(x), \quad \mu = \frac{mm'}{m+m'}. \quad (13)$$

Similarly we can express  $\langle V \rangle_{S_0}$  as:

$$\begin{aligned} \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \langle V \rangle_{S_0} &= \sum_k |c_k|^2 \int_0^\beta d\tau e^{-\omega_k \tau} e^{-k^2 \tau / 2(m+m')} \\ &\times \sum_{n=0}^{\infty} e^{-(\varepsilon_n - \varepsilon_0) \tau} \int U_0^*(x_1) U_n(x_1) U_n^*(x_2) U_0(x_2) e^{i\mu k(\underline{x}_1 - \underline{x}_2)} d^3x_1 d^3x_2. \end{aligned} \quad (14)$$

Using (3), (4), (10) and (14) we can represent the total energy functional  $\Phi_1$  as:

$$E_0 \leq \Phi_1 \quad (15)$$

$$\begin{aligned} \Phi_1 &= -\frac{1}{2\mu} \int U_0^* \Delta U_0 d^3x - \frac{e^2 \omega_p^2}{4\pi^2} \int d^3k \frac{1}{k^2 \omega_k} \\ &\times \sum_n \int e^{i\mu k(\underline{x}_1 - \underline{x}_2)} \frac{U_0^*(\underline{x}_1) U_n(\underline{x}_1) U_n^*(\underline{x}_2) U_0(\underline{x}_2)}{\omega_k + [k^2/2(m+m')] + \Delta\varepsilon_n} d^3x_1 d^3x_2 \end{aligned} \quad (16)$$

$$\Delta\varepsilon_n = \varepsilon_n - \varepsilon_0 \geq 0 \quad (17)$$

Thus the minimum of the functional  $\Phi_1$  gives the upper limit of the ground state.

### 3. Numerical Calculations of the Self-Energy

The exact solution of the general problem is too complicated and requires the solution of the nonlinear variational functional (16) for  $U_0(x)$  together with the Schrödinger equation defined by the Hamiltonian (13) and the condition

$$\frac{\partial \Phi_1}{\partial \mu} = 0. \quad (18)$$

Note that we make inequality (10) even stronger, if we confine the sum over  $n$  in (16) only by the first term. In this case we have from (16):

$$\begin{aligned} \Phi_1 &= -\frac{1}{2\mu} \int U_0^* \Delta U_0 d^3x - \frac{e^2 \omega_p^2}{4\pi^2} \int d^3k d^3x_1 d^3x_2 \\ &\times \frac{|U_0(x_1)|^2 |U_0(x_2)|^2}{k^2 \omega_k [\omega_k + k^2/2(1+m')]} e^{i\mu k(\underline{x}_1 - \underline{x}_2)}. \end{aligned} \quad (19)$$

The exact calculation of (19) is still too complicated, and for its estimation we choose the Gauss probe wave function

$$U_0(x) = \frac{l^{3/2}}{\pi^{3/4}} \exp\left(-\frac{l^2 x^2}{2}\right). \quad (20)$$

Substituting (20) into (19) and using the relations

$$\hbar\omega_p = \sqrt{12}r_s^{-3/2} \text{Ry}, \quad r_s = \left(\frac{9\pi}{4}\right)^{1/3} \frac{1}{k_F a_0}, \quad (21)$$

where Ry = 13.6 eV is the Rydberg constant,  $k_F$  is the Fermi impuls and  $a_0$  is the Bohr radius. From (19) we obtain

$$\begin{aligned} \frac{\Phi_1}{\text{Ry}} = & \frac{3}{2\mu} B^2 - \frac{2}{\pi} \sqrt[3]{12} r_s^{-3/4} \int_0^\infty dx \frac{\exp[-\sqrt{3} r_s^{-3/2} \mu^2 (x^2/B^2)]}{\sqrt{1 + \left(\pi^{2/3} / \sqrt[3]{3} \sqrt[3]{2} \sqrt{r_s}\right) x^2 + x^4}} \\ & \times \frac{1}{\sqrt{1 + \left(\pi^{2/3} / \sqrt[3]{3} \sqrt[3]{2} \sqrt{r_s}\right) x^2 + x^4 + (1 - \mu)x^2}}. \end{aligned} \quad (22)$$

Expression (22) should be minimized with respect to the two parameters  $B \in (0, \infty)$  and  $\mu \in (0, 1)$ , where  $B$  is connected with  $l$  in (20) by the relation  $B = la_0$ . Thus the physical meaning of the value  $B^{-1}$  is the effective radius of the electron state defined by the variational probe function (20).

The dependence of  $B$  on  $r_s$  is represented in Fig. 1. From this figure it can be seen that the region  $(0, r_{sc})$  corresponds to the stable delocalized electron state (solid line). In this region the value of  $\mu$  is approximately zero, according to weak coupling (Fig. 1(b), solid line). At the critical value  $r_{sc} = 418$  the effective radius of the electron decreases abruptly and becomes finite. In the region  $(r_{sc}, \infty)$  the electron is self-trapped in a stable state. This corresponds to the case of strong coupling with  $\mu = 1$  (solid line in Fig. 1(b)). With increasing  $r_s$  in the region  $(r_{sc}, \infty)$  the effective radius of the electron state also increases and becomes infinite in the limit of  $r_s \rightarrow \infty$ . This corresponds to the limit of zero electron densities.

Figure 1(c) illustrates the dependence of the ground state energy on  $r_s$ . The solid line in this figure corresponds to the total energy of stable delocalized electron states in the region  $(0, r_{sc})$  and metastable delocalized states in the region  $(r_{sc}, \infty)$ . The point  $r_{sm}$  is the critical point where the metastable state originates, its value is  $r_{sm} = 71$ . In the region  $(r_{sm}, r_{sc})$  this metastable state is shown in Fig. 1(c) by the dashed line. According to Fig. 1(b) this state corresponds to the strong coupling case where  $\mu = 1$ . From Fig. 1(a) it can be seen, that the effective radius of the electron in the metastable region  $(r_{sm}, r_{sc})$  is finite (dashed line in Fig. 1(c)), in the region  $(r_{sc}, \infty)$ , this corresponds to the self-trapped electron state and to finite values of the electron effective radius (solid line in Fig. 1(a) in the region  $(r_{sc}, \infty)$ ).

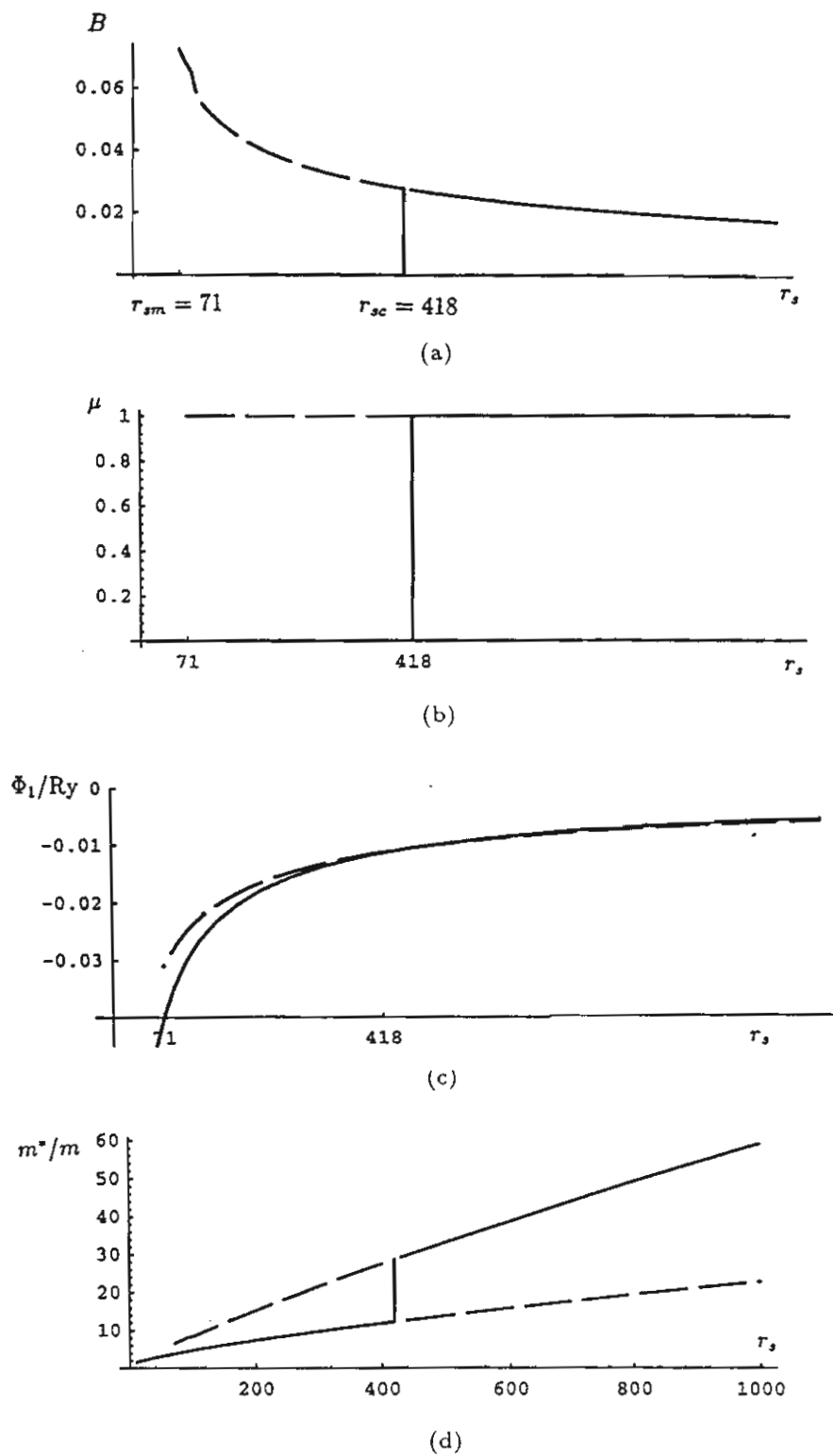


Fig. 1.

The metastable state in the region  $(r_{sc}, \infty)$  is in order to the delocalized state (solid line in Fig. 1(c)) and to the localized state in the region  $(r_{sm}, r_{sc})$  (dashed line in Fig. 1(c) in this region).

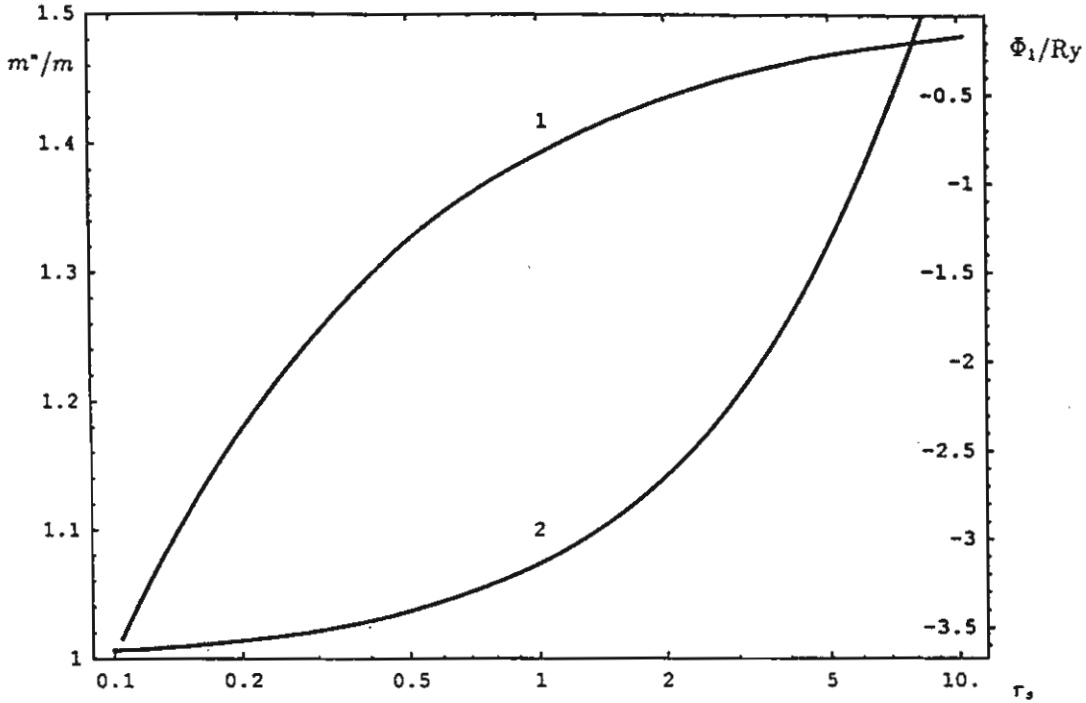


Fig. 2. The dependence of the self-energy  $\Phi_1/Ry(1)$  and the effective mass  $m^*/m(2)$  on  $r_s$ .

In Fig. 2 we present the  $\Phi_1/Ry$  dependence on  $r_s$  in the interval  $(0.1, 10)$  which is appropriate to real densities of metals (line 1).

#### 4. Effective Mass

According to Refs. 10 and 11 the effective mass of the plasmaron can be obtained from the modified expression of the total energy (8) generalized to the case of a moving electron:

$$E_0 = - \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \int_{\underline{r}(\beta) = \underline{r}(0) + \beta \underline{u}} e^{-S[\underline{r}]} D\underline{r} \quad (23)$$

where  $\underline{u} = i\underline{v}$  is the complex velocity of the particle. In the limit of small velocities it follows from (23):

$$E_0 = E_{0,0} + \frac{m^* v^2}{2} + \dots \quad (24)$$

where  $m^*$  is the effective mass of the particle. The value  $E_{0,0}$  is the ground state energy for the rest particle and was calculated above. Using the results of Refs. 10 and 11 we obtain from (23) and (24) the expression for the effective mass in

self-consistent approximation:

$$m^* = m + \frac{2}{3} \sum_k |c_k|^2 \frac{k^2}{[\omega_k + (k^2/2)(1 - \mu)]^3} \left| \int |u_0(x)|^2 e^{i\mu kx} d^3x \right|^2 \quad (25)$$

where the wave function must be chosen according to the minimization of the functional (19).

In the case of weak coupling  $\mu \rightarrow 0$ , which corresponds to the limit of high densities  $r_s \rightarrow 0$ , it follows from (5) and (25):

$$\frac{m^*}{m} = 1 + \frac{2}{3} r_s^{3/2}. \quad (26)$$

In the case of strong coupling  $\mu \rightarrow 1$ , which corresponds to the limit of low densities  $r_s \rightarrow \infty$ , it follows from (5) and (25):

$$\frac{m^*}{m} = 1 + \frac{\pi}{2\sqrt[3]{3}} r_s^{3/4}. \quad (27)$$

## 5. Numerical Calculation of the Effective Mass

Substituting (20) into (25) we get from (25) the expression for the effective mass in the form:

$$\begin{aligned} \frac{m^*}{m} = 1 + \frac{2}{9} 12^{3/4} r_s^{3/4} \int dx x^2 \frac{1}{\sqrt{1 + \left( \pi^{2/3} / \sqrt[3]{3} \sqrt[3]{2} \sqrt{r_s} \right) x^2 + x^4}} \\ \times \frac{\exp \left( -\sqrt{3} \mu^2 r^{-3/2} x^2 / B^2 \right)}{\left( \sqrt{1 + \left( \pi^{2/3} / \sqrt[3]{3} \sqrt[3]{2} \sqrt{r_s} \right) x^2 + x^4} + (1 - \mu)x^2 \right)^3} \end{aligned} \quad (28)$$

where the parameters  $B$  and  $\mu$  are taken from the solution of the minimizing problem (22) and are presented in Fig. 1(a) and 1(b). The results of the numerical calculations are presented in Fig. 1(d). At the critical point  $r_{sc}$  the effective mass abruptly increases with increasing  $r_s$ . This corresponds to the transition from the limit of weak coupling to strong coupling. This behavior follows from the self-consistent approximation. If we take the excited states of the Hamiltonian (13) into account, the expression for the effective mass  $\tilde{m}^*$  is:

$$\tilde{m}^* = m^* + \Delta m \quad (29)$$

where

$$\begin{aligned} \Delta m = \sum_{n=1}^{\infty} \sum_k |c_k|^2 \frac{k^2}{[\omega_k + (k^2/2)(1 - \mu) + \Delta \varepsilon_n]^3} \\ \times \int U_0^*(x_1) U_n(x_1) U_n^*(x_2) U_0(x_2) e^{i\mu k(\underline{x}_1 - \underline{x}_2)} d^3x_1 d^3x_2 \end{aligned} \quad (30)$$

From (29) and (30) it follows that  $\Delta m > 0$ , so the obtained results in the self-consistent approximation give the lower bound of the effective mass.

In Fig. 2 we present the plot for the effective mass obtained in the self-consistent approximation in the range of  $r_s \in (0.1, 10)$ , which is appropriate to real metals (line 2).

## 6. Comparison with Experimental Data

The obtained results can be used to calculate the bandwidth of electrons in metals. Figure 2 shows the numerical estimation of the bottom of the electron band. The upper edge of the band was calculated in a lot of other papers. For a review see Ref. 4 and references therein. From these calculations it follows that the upper edge of the electron band can be approximated by the Hartree-Fock approach with sufficient accuracy. In this approximation we have:

$$\mu - \varepsilon_F = -\frac{2}{\pi} \left( \frac{9\pi}{4} \right)^{1/3} \frac{1}{r_s} \text{Ry} \approx -\frac{1.22}{r_s} \text{Ry} \quad (31)$$

Thus the width of the conduction band is equal to  $\Delta = \mu - \Phi_1$  where  $\Phi_1$  is defined by (22).

The table presents the values of  $r_s$ ,  $\Phi_1$ ,  $\mu - \varepsilon_F$ ,  $\Delta$  and experimental values for the bandwidth  $\Delta_{\text{exp}}$  obtained for a few metals by the method of soft X-ray emission.

|                                           | Li    | Na    | Be    | Mg    | Al    |
|-------------------------------------------|-------|-------|-------|-------|-------|
| $r_s$ [Ref. 4]                            | 3.26  | 4.00  | 1.88  | 2.66  | 2.07  |
| $\Phi_1/\text{Ry}$ (22)                   | -0.36 | -0.32 | -0.53 | -0.42 | -0.5  |
| $(\mu - \varepsilon_F)/\text{Ry}$ (31)    | -0.37 | -0.31 | -0.65 | -0.45 | -0.59 |
| $\Delta/\text{Ry}$                        | 0.317 | 0.247 | 0.93  | 0.49  | 0.77  |
| $\Delta_{\text{exp}}/\text{Ry}$ [Ref. 12] | 0.27  | 0.26  | 1.00  | 0.46  | 0.87  |

This table demonstrates a good agreement between the theoretical and experimental values.

## 7. Discussion

The obtained numerical results for the electron-plasmon interaction illustrate the behavior of the electron ground state for a wide range of the electron-plasmon coupling. In the region where  $r_s$  is appropriate to the density of real metals, where the perturbation theory requires the summation of an infinite number of diagrams, the developed path integral approach can be used as the basis for the calculation of the electronic properties of such systems.

We would like to stress that the obtained results are only valid within the self-consistent approximation. More precise results can be obtained if the excited states of the Hamiltonian (13) is taken into account.

## ***APPENDIX 3***

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23 June 1998

Dr. V. Sa-yakanit  
Forum for Theor. Sci.  
Physics Dept. Fac. Sci.  
Chulalongkorn  
Bangkok 10330, THAILAND

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Path-integral approach to the electron density of  
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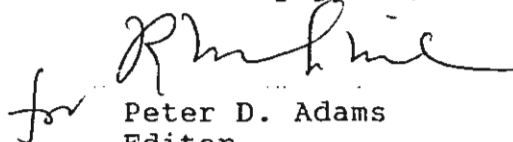
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| THIRD AUTHOR:               |                                                                                                                |
| CORRESPONDING AUTHOR:       | DR. V. SA-YAKANIT<br>FORUM FOR THEOR. SCI.<br>PHYS DEPT. FAC. SCI.<br>CHULALONGKORN<br>BANGKOK 10330, THAILAND |
| TELEPHONE:                  | 011 66 2 251 7300                                                                                              |
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# Path-integral approach to the electron density of states at the interface of a single modulation-doped heterojunction

V. Sa-yakanit

Forum for Theoretical Science, Department of Physics, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

G. Slavcheva

Institute of Biophysics, Bulgarian Academy of Sciences, Acad. G. Bontchev Street bl.21, 1113 Sofia, Bulgaria

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The electronic density of states (DOS) at the interface of a single modulation-doped heterojunction is calculated both in the fluctuation band tail and in the semiclassical limit using the path-integral method. Due to charge density inhomogeneities in the heavily doped barrier region, random potential fluctuations are generated in whose minima carriers are localized, resulting in a band-tail density spectrum. The screening of the long-range potential fluctuations, which are important for the problem considered, is accounted for by using the two-dimensional Thomas-Fermi model. The statistical properties of the random impurity charge distribution are taken into account using the binary correlation function of the random potential for the specific geometry of the problem in two limiting cases of the general correlation function. Analytical expressions for the dimensionless functions of the exponential and preexponential of the band-tail DOS, as a function of the energy, are obtained in the weak and strong screening limit for the quasi-2D case under consideration and are compared to the respective functions for the general  $d$ -dimensional case. The dependence of the band-tail DOS behavior on the relevant parameters of the system, namely, spacer layer thickness, doping layer thickness, 2D EG thickness, and 3D-impurity concentration is studied numerically for  $\text{Al}_x\text{Ga}_{1-x}\text{As}$ -GaAs modulation doped heterostructures and numerical results for the 2D-DOS are presented. The band-tail results for the 2D-DOS are compared with the Kane approximation derived by taking the limit  $\epsilon \rightarrow 0$  in order to determine  $\rho(E)$  in the whole energy range. We compare the results from the two computed cases of the path-integral expression for the DOS corresponding to the two limits of the general correlation function with each other. On the other hand, we compare the semiclassical limit and the white Gaussian noise limit of the above results with many other theoretical methods such as the generalized semiclassical method, multiple scattering method and the simulations resulting from the tight-binding model. [S0163-1829(98)04836-X]

## I. INTRODUCTION

It is well known that charge impurities play an essential role in determining the electronic, optical, and transport properties of the quantum wells (QW) and heterostructures (HS). Thus they are of great significance for the device performance characteristics based on them. In modulation-doped heterostructures, the charged donor centers are placed at a finite distance from the interface in order to reduce the ionized impurity scattering at low temperatures that we claim to be a major scattering mechanism, limiting the electron mobility in such structures. Since these remote ions act as a necessary supplier of electronic space charge in the well material, the impurity scattering is in principle unavoidable and unlike the other scattering mechanisms whose influence can be reduced by technological improvements. It is frequently considered as an inherent limit to the mobility. In Fig. 1 the band diagram of the modulation-doped GaAs- $\text{Al}_x\text{Ga}_{1-x}\text{As}$  heterojunction is shown.

Electrons confined to the narrow potential well in the well material (e.g., GaAs at the interface of the GaAs/ $\text{Al}_x\text{Ga}_{1-x}\text{As}$  heterostructure) form a quasi-two-dimensional electron gas (2D EG). Quantization of the electronic motion perpendicular to the interface leads to a series of 2D electric quantum limit subbands,  $E_i$  ( $i=0,1,2,\dots$ ), each corresponding to a quantized energy level of the potential well.

The charged donors are randomly distributed in the highly doped region and the charge density fluctuates about its mean value. This in turn generates potential fluctuations at or near the interface of the heterojunction in whose minima carriers can be localized resulting in a band-tail density of states spectrum. A similar band-tailing phenomenon has been considered for the MIS heterostructures in Ref. 1. On the other hand the 2D electrons are scattered by the potential fluctuations at the interface, thereby determining the electron mobility. As has been pointed out in Ref. 2 an important feature of the problem is that the 2D electrons are affected

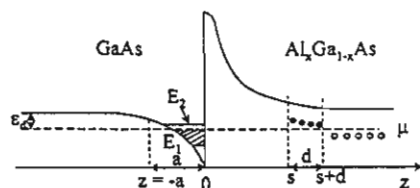


FIG. 1. Band diagram of a single GaAs/ $\text{Al}_x\text{Ga}_{1-x}\text{As}$  heterojunction. The solid line represents the discontinuity of the conduction-band edge profile near the interface. The horizontal dashed line represents the chemical potential of the system  $\mu$ .  $E_d$  is the bound energy of donor levels.  $\bullet$ : levels of the charged donors;  $\circ$ : levels of the neutral donors;  $E_1$ ,  $E_2$  are correspondingly the ground-state energy and the first excited state energy of the potential well at the interface; the electronic states occupied by the 2D EG are patterned.

only by the fluctuations of the concentration of the charged donors with a characteristic size of the same order or greater than the width of the spacer layer  $s$ . The potential of the short-wavelength fluctuations exponentially decays with the increase of the distance from the charged donors' layer. It should be noted that the random potential can result not only from the charge density inhomogeneity but can also be due to the fact that the charged donors are not located in the same plane. In the case of  $\delta$ -doped layers this mechanism is absent but in the case of thick doped layers, as will be shown below, this mechanism plays an important role.

In this paper we assume that  $s$  is much greater than the average distance between the charged donors. Also we shall consider only the large-scale fluctuations of the random potential generated by the surface charge density fluctuations of the impurities forming a highly doped layer in the barrier material of the heterostructure. The electrons at the interface move in a random impurity potential which represents a disordered environment.

It has been pointed out in Ref. 3 that although the total impurity distribution obeys Poisson's law, if part of the donors in the layer are neutral, a correlation in the spatial distribution of the charged donors occurs. This is due to the Coulomb interaction between the charged impurities. This correlation appreciably lowers the potential fluctuations, which in turn result in an enhancement of the calculated mobility of the 2D EG as has been shown in Ref. 4 in accordance with mobilities reported to date (see, e.g., Ref. 5).

The aim of the present study is to analyze the influence of the fluctuation of the positively charged centers' density in the highly doped barrier region on the spectrum of the interface states resulting in band tailing phenomena. The disorder is represented by the statistical properties of the spatial distribution of the charged impurities, characterized by its moments and in particular by the binary correlation function. Various models of the correlation function are available.<sup>3,6</sup> In what follows we shall adopt the expression for the binary correlation function (variance) of the random potential derived in Ref. 7 as the most appropriate for the geometry of the problem considered. The screening of the impurities by the 2D EG is evaluated in a generalized Thomas-Fermi approximation<sup>7</sup> considering a small but finite width of the 2D EG with a uniform electron density along the  $z$  coordinate perpendicular to the interfacial plane. A possible model could be the correlation function derived by using Fang and Howard's variational function,<sup>8</sup> which, as we have proved, leads to more cumbersome expression. Nevertheless our choice has been dictated by the possibility of obtaining analytical expressions for the DOS, whose physical interpretation could be more transparent. The problem of density of the localized electron states in the band tail at the interface of the heterojunction has been treated within the framework of the Feynman path-integral approach<sup>9</sup> in which a nonlocal harmonic oscillator trial action has been introduced.

In this paper we obtain analytical expressions for the DOS of the first conduction subband edge deep in the band tail in two limiting cases of the general correlation function. These closely model the realistic physical situation. We obtain asymptotics for the dimensionless functions of the preexponential factor  $a(\nu)$  and the exponential  $b(\nu)$ , respectively, for the weak screening and strong screening case and study the

dependence of the logarithmic derivative of the latter (or the power, if the power law is assumed) on the dimensionless energy  $\nu$ . Numerical calculations of the DOS in the band tail are made for a single GaAs-Al<sub>x</sub>Ga<sub>1-x</sub>As modulation-doped heterojunction varying the relevant parameters, namely, the impurity concentration, the spacer layer thickness, the doped layer thickness and the 2D EG thickness. A comparison between the two DOS expressions corresponding to the two limits of the general correlator has been performed and their behavior on the relevant system parameters has been numerically studied. In order to be able to compare the obtained results in the whole energy range, we have taken the semiclassical Kane limit  $\epsilon \rightarrow 0$  of the path-integral expression for the DOS, which corresponds to large energies and we have derived semiclassical analytical expressions of the DOS for the quasi-2D problem considered. We have compared our results with different theoretical approaches for the calculation of the 2D DOS near the first conduction-band edge. We have obtained complete correspondences between our semiclassical result for the 2D DOS and the generalized semiclassical model described in Ref. 10. Our band tail and semiclassical DOS results have been compared with the band-edge DOS calculations<sup>11</sup> using the multiple-scattering method, which includes a finite-range screened potential and an impurity concentration to all orders. Finally, the white Gaussian noise limit of our result for the DOS has been compared with the tight-binding simulations of the 2D white Gaussian noise problem, the fluctuation theory calculations of Ref. 12, and the results calculated from the coherent potential approximation (CPA). A very good agreement between the band-tail DOS, obtained by using the path-integral method and the tight-binding calculations, has been found in contrast with the fluctuation theory results.

The outline of the paper is as follows: In Sec. II we give the statement of the problem; we assume a Thomas-Fermi screening model and we reformulate it in terms of the path-integral technique. We also derive analytical asymptotic expressions for the DOS in the band tail of the first conduction subband within the first cumulant approximation. In Sec. III we obtain analytically the asymptotics of the dimensionless functions in the preexponent  $a(\nu)$  and exponential  $b(\nu)$ , respectively, in the weak screening and strong screening cases and compare the energy dependence with the general  $d$ -dimensional case results for other model fluctuating potentials (Gaussian and screened Coulomb). In Sec. IV we present numerical results for the band-tail DOS applied to the single GaAs-Al<sub>x</sub>Ga<sub>1-x</sub>As modulation-doped heterojunction. We study the behavior of the power of the power-law energy dependence of the exponential in the DOS as a function of the dimensionless energy as well as the behavior of the DOS altering the important physical parameters of the system, namely, the 3D-impurity doping concentration, spacer layer thickness, doped layer thickness and 2D EG thickness. In Sec. V we derive the semiclassical limit of our path-integral result for the DOS and compare it with the band-tail DOS results as well as with the two DOS expressions corresponding to the two limiting cases of the general correlation function, varying the disorder parameter (represented by the dispersion of the random potential), the spacer layer thickness and the 2D EG thickness. In Sec. VI we compare our results for the DOS with the generalized semi-

classical approach,<sup>10</sup> multiple-scattering method,<sup>11</sup> and tight-binding numerical simulation and the fluctuation theory results.<sup>12</sup> The conclusions of the work are summarized in Sec. VII.

## II. STATEMENT OF THE PROBLEM

We shall assume that the charged donors are distributed in the highly doped region with a thickness  $d$  in a purely random fashion with a concentration  $n_I$  (Fig. 1) at a distance  $s$  from the interface, that is the impurity charge density obeys Poisson's law. Following Ref. 7 we adopt the generalized two-dimensional Thomas-Fermi screening model. Our purpose is to obtain the electron-ion interaction potential  $v(r)$ , where  $r=(x,y)$  is the 2D in-plane coordinate at the interfacial plane in order to calculate the 2D-binary correlation function of the random potential. This has been done in Ref. 7 solving the 2D Poisson equation for the potential  $\Phi(z)$  seen by the electrons due to an external charge density  $\rho_{\text{ext}}(r,z)$  using the important assumption that there exists a decomposition of the 3D number density into a 2D component  $n_I(r)$  in the interfacial plane and a density  $f(z)$  along the  $z$  axis perpendicular to the plane, which reads

$$N_V(r,z) = n_I(r)f(z). \quad (1)$$

We shall assume that the 2D EG has a small but finite width  $a$  and take  $f(z)$  as being uniform along the  $z$  axis, i.e.,  $f(z) = 1/a$ ,  $-a \leq z \leq 0$  (see Fig. 1), or equivalently

$$f(z) = \frac{1}{a} [\theta(z+a) - \theta(z)]. \quad (2)$$

We have shown, following the same procedure for determining the correlation function,<sup>7</sup> that the expressions obtained by using the variational wave function of Fang and Howard (or equivalently the density function being the square of the wave function) instead of the above function lead to more complex results whose physical meaning is not quite transparent and any further calculations become extremely cumbersome. This is the reason for choosing the above simple uniform density function.

We shall not give here details of the calculations (for which we refer to Ref. 7) but only briefly mention the main assumptions and results. Defining the mean 2D electric potential  $\bar{\Phi}(r)$  independent of  $z$  according to

$$\bar{\Phi}(r) = \int_{-\infty}^{\infty} dz \Phi(r,z)f(z) \quad (3)$$

and using the Thomas-Fermi approximation, Poisson's equation is obtained in the form

$$-\nabla^2 \Phi(r,z) + 2q_s f(z) \Phi(r) = \frac{1}{4\pi\epsilon_0\epsilon_s} \rho_{\text{ext}}(r,z) \quad (4)$$

where  $\epsilon_s$  is the dielectric constant in the heterostructure (assumed to be equal in both materials),  $\epsilon_0$  is the dielectric permittivity of the vacuum, and the 2D inverse screening length has been introduced according to the following equation:

$$q_s = \frac{a}{2} Q_s^2 \quad (5)$$

where  $Q_s$  is the 3D Thomas-Fermi screening wave vector. Equation (4) has been solved using the Fourier transform technique, and after introducing the dielectric function

$$\epsilon(q) = 1 + \frac{q_s}{q} F(q), \quad (6)$$

we get that

$$\bar{\Phi}(q) = \frac{1}{\epsilon(q)} \bar{\Phi}_{\text{ext}}(q), \quad (7)$$

where  $F(q)$  is the form factor, which for this particular choice of  $f(z)$  is given by

$$F(q) = \frac{2}{(qa)^2} (e^{-qa} + qa - 1). \quad (8)$$

For the 2D electron-impurity potential the following expression is obtained:

$$v(q) = - \left( \frac{Ze^2}{8\pi\epsilon_0\epsilon_s a} \right) \frac{(1 - e^{-qa})e^{-qZ_i}}{q^2 \epsilon(q)}, \quad (9)$$

where  $Z=1$  for the monovalent impurity center and  $Z_i$  is the distance of the impurity center to the interfacial plane. The binary correlation function is defined as follows:

$$W(r-r') = n_I \int dZ_i \int d^2R_i v(r-R_i) v(r'-R_i). \quad (10)$$

Finally, for the Fourier transform of the 2D binary correlation function a general expression has been derived, namely,

$$W(q) = n_I \left( \frac{Ze^2}{8\pi\epsilon_0\epsilon_s a} \right)^2 \frac{e^{-2qs} (1 - e^{-2qd})(1 - e^{-qa})^2}{q^4 [\epsilon(q)]^2} \quad (11)$$

where  $s$  is the spacer layer thickness,  $d$  is the highly doped region thickness, and  $\epsilon(q)$  is given by Eqs. (6) and (8).

The possible limits of the binary correlation function have been derived in Ref. 7 and we shall consider only the two limits corresponding to a wide spacer ( $sq_s \gg 1$ ) since they are relevant to the real physical situation.

In contrast to the statement in Ref. 7 that the doped region thickness  $d$  is not important, we found that eliminating the  $d$  dependence leads to divergencies because of the wave-vector  $q$  dependence, therefore in what follows we shall keep the term containing  $d$ . In case 1 corresponding to a wide spacer layer:  $sq_s \gg 1$  and thin 2D EG layer:  $aq_s \ll 1$ :

$$W(q) = n_I b^2 a^2 \frac{e^{-2qs} (1 - e^{-2qd})}{2q (q + q_s)^2} \quad (12)$$

and in case 2: a wide spacer layer:  $sq_s \gg 1$  and thick 2D EG layer:  $aq_s \gg 1$ :

$$W(q) = n_I b^2 \frac{e^{-2qs} (1 - e^{-2qd})}{2q (q^2 + Q_s^2)^2} \quad (13)$$

where

$$b = \frac{Ze^2}{8\pi\epsilon_0\epsilon_r a}. \quad (14)$$

Let now reformulate the problem of the electronic DOS calculation in terms of the path-integral method.<sup>9</sup> As the origin of the disorder the fluctuation potential relief generated by the remote randomly distributed charged impurity centers is assumed. The electron motion at or near the disordered interface of the heterojunction in the field of  $N$  charged impurity centers confined in a volume  $V$  in the highly doped region with a thickness  $d$  with 3D density  $n_I = N/V$  and surface density  $n_I d$  is described by the Hamiltonian

$$H = -\frac{\hbar^2}{2m^*} \nabla^2 + \sum_i \nu(\mathbf{r} - \mathbf{R}_i), \quad (15)$$

where the individual impurity potential  $\nu(\mathbf{r} - \mathbf{R}_i)$  generated at a point  $\mathbf{r}(x, y)$  in the heterojunction interfacial plane by impurity ions positioned at a point  $(\mathbf{R}_i, Z_i)$  ( $\mathbf{R}_i$  being the impurity in-plane coordinate) can be identified with the 2D electron-impurity potential from Ref. 9. The DOS per unit volume can be expressed in terms of the diagonal elements of the one-electron propagator of the electron moving in the field of  $N$  impurities as

$$\rho(E) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt e^{(i/\hbar)Et} \bar{G}(0,0;t). \quad (16)$$

According to Ref. 9, the problem of the DOS calculation is reduced to obtain the average (over all impurity configurations) one-electron propagator:

$$\bar{G}(\mathbf{r}_2, \mathbf{r}_1; t) = \int D[\mathbf{r}(\tau)] e^{(i/\hbar)S}, \quad (17)$$

where the boundary conditions are given by  $\mathbf{r}(0) = \mathbf{r}_1, \mathbf{r}(t) = \mathbf{r}_2$  and  $S$  is the action of the random system, given by

$$S = \int_0^t d\tau \left[ \frac{m^*}{2} \dot{\mathbf{r}}^2(\tau) - E_0 + \frac{i}{2\hbar} \int_0^t d\sigma W[\mathbf{r}(\tau) - \mathbf{r}(\sigma)] \right]. \quad (18)$$

Here we have limited the expansion over the subsequent moments of the random potential distribution up to the second-order moment (binary correlator). The mean potential energy and the binary correlation functions are given by

$$n_I \int d\mathbf{R} \nu(\mathbf{r} - \mathbf{R}) = E_0, \quad (19)$$

$$n_I \int d\mathbf{R} \nu(\mathbf{r} - \mathbf{R}) \nu(\mathbf{r}' - \mathbf{R}) = W(\mathbf{r} - \mathbf{r}').$$

Furthermore, following Ref. 9, the full action is approximated by a nonlocal harmonic oscillator action (the so-called "trial" action), depending on the variational parameter  $\omega$ , which is given by

$$S_0 = \int_0^t d\tau \left[ \frac{m^*}{2} \dot{\mathbf{r}}^2(\tau) - \frac{\omega^2}{2t} \int_0^t d\sigma |\mathbf{r}(\tau) - \mathbf{r}(\sigma)|^2 \right], \quad (20)$$

which corresponds to a zero-order approximation  $\bar{G}_0$  to  $\bar{G}$ .

The average propagator may be written in terms of the trial action as

$$\bar{G} = \bar{G}_0 \langle e^{(i/\hbar)(S - S_0)} \rangle_{S_0} \quad (21)$$

by using the path-integral normalization. By keeping only the first-order cumulant, the first-order approximation to  $\bar{G}$  is obtained as

$$\bar{G}_1 = \bar{G}_0 \exp \left( \frac{i}{\hbar} \langle S - S_0 \rangle_{S_0} \right). \quad (22)$$

The diagonal part of  $\bar{G}_1$  in the 2D case we are considering leads to the following expression for the DOS:

$$\begin{aligned} \rho_1(E) = & \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \left( \frac{m^*}{2\pi i \hbar t} \right) \left( \frac{\omega t}{2 \sin \omega t/2} \right)^2 \\ & \times \exp \left[ -\frac{i}{\hbar} (E_0 - E)t - \frac{\xi}{2\hbar^2} \frac{t}{2\pi} \right. \\ & \times \int_0^t dx \int \frac{d^2 q}{(2\pi)^2} W(q) e^{-Aq^2 + i\mathbf{q} \cdot \mathbf{B}} \\ & \left. - \frac{1}{2} \left[ \frac{\omega t}{2} \cot \left( \frac{\omega t}{2} \right) - 1 \right] \right], \end{aligned} \quad (23)$$

where  $W(q)$  is given by Eq. (11),  $\xi$  is the dispersion of the random potential energy, and the functions  $A$  and  $B$  have been defined (see Ref. 13 for the 3D case derivation) for the 2D case, according to

$$A = \frac{1}{2} \left\{ \frac{1}{2} \langle [\mathbf{r}(\tau) - \mathbf{r}(\sigma)]^2 \rangle_{S_0(\omega)} - \langle [\mathbf{r}(\tau) - \mathbf{r}(\sigma)] \rangle_{S_0(\omega)}^2 \right\}, \quad (24)$$

$$\mathbf{B} = \langle \mathbf{r}(\tau) - \mathbf{r}(\sigma) \rangle_{S_0(\omega)}. \quad (25)$$

The above averages over the trial action can be calculated by taking the functional derivatives of the characteristic functional

$$\left\langle \exp \left( \frac{i}{\hbar} \int_0^t d\tau \mathbf{f}(\tau) \cdot \mathbf{r}(\tau) \right) \right\rangle_{S_0(\omega)},$$

analogously to the derivation in 3D (see Ref. 13).

Since in order to calculate the DOS we need only the diagonal part of  $\bar{G}_1(\mathbf{r}_2, \mathbf{r}_1; t, \omega)$ , we can set  $\mathbf{r}_2 = \mathbf{r}_1$ , which directly leads to  $\mathbf{B} = 0$  and considerably simplifies Eq. (23).

In order to evaluate the ground-state energy contribution to the DOS we take the limit  $t \rightarrow \infty$ . This leads to the following expression for  $A$ :

$$A \approx \frac{3\hbar}{4m^* \omega} \quad (26)$$

and the DOS asymptotic expression:

$$\rho_1(E) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \left( \frac{m^*}{2\pi i \hbar t} \right) (i\omega t)^2 \times \exp \left[ -\frac{1}{2} i\omega t - \frac{i}{\hbar} (E_0 - E)t - \frac{\xi}{2\hbar^2} \frac{t^2}{2\pi} \int \frac{d^2 q}{(2\pi)^2} W(q) e^{-Aq^2} \right]. \quad (27)$$

Let us consider now the expressions corresponding to both limiting cases [Eqs. (12) and (13)] obtained for the 2D binary correlation function. In the first case ( $sq_s \gg 1, aq_s \ll 1$ ) we expand the term containing the dependence on the doped layer thickness  $d$  up to the linear term, thus obtaining

$$W(q) \approx n_I b^2 a^2 d \frac{e^{-2q_s}}{(q + q_s)^2}. \quad (28)$$

In the second case of a relatively thick 2D EG layer ( $sq_s \gg 1, aq_s \gg 1$ ), analogously we get

$$W(q) \approx n_I b^2 d \frac{e^{-2q_s}}{(q^2 + Q_s^2)^2}. \quad (29)$$

It is possible to perform exactly the integration over the 2D wave vector in Eq. (27) and we get the following expression for the DOS in the two cases considered:

$$\rho_1(E) = \begin{cases} \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \left( \frac{m^*}{2\pi i \hbar t} \right) (i\omega t)^2 \exp \left[ -\frac{1}{2} i\omega t - \frac{i}{\hbar} (E_0 - E)t - \frac{\xi'}{2\hbar^2} \frac{t^2}{2\pi} (e^{-Aq_s^2} - 1) \right] \times \left[ \frac{1}{(2sq_s)^2} - \frac{1}{2sq_s} \left( \frac{Aq_s}{s} - 1 \right) \right] + \frac{1}{2sq_s}, & sq_s \gg 1, aq_s \ll 1 \\ \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \left( \frac{m^*}{2\pi i \hbar t} \right) (i\omega t)^2 \exp \left[ -\frac{1}{2} i\omega t - \frac{i}{\hbar} (E_0 - E)t - \frac{\xi''}{2\hbar^2} \frac{t^2}{2\pi} \left[ 1 - 2Q_s^2 \left( Aw + \frac{su}{Q_s} \right) \right] \right] \times e^{AQ_s^2 - \frac{A}{2s^2}}, & sq_s \gg 1, aq_s \gg 1, \end{cases} \quad (30)$$

where the following quantities representing the dispersion of the random potential energy and having the dimension of energy squared, have been introduced:

$$\xi' = n_I d a^2 \left( \frac{Ze^2}{8\pi\epsilon_0\epsilon_s a} \right)^2 \quad (31)$$

and

$$\xi'' = \frac{n_I d}{2Q_s^2} \left( \frac{Ze^2}{8\pi\epsilon_0\epsilon_s a} \right)^2 \quad (32)$$

and for the second case the following functions:

$$u = \text{ci}(2sQ_s) \sin(2sQ_s) - \text{si}(2sQ_s) \cos(2sQ_s) \quad (33)$$

$$w = -\text{ci}(2sQ_s) \cos(2sQ_s) - \text{si}(2sQ_s) \sin(2sQ_s).$$

For both cases considered we can introduce, analogously to Ref. 9, the dimensionless variable

$$z = \begin{cases} \frac{3}{2} \frac{E_{q_w}}{E_w}, & sq_s \gg 1, aq_s \ll 1 \\ \frac{3}{2} \frac{E_{Q_s}}{E_w}, & sq_s \gg 1, aq_s \gg 1, \end{cases} \quad (34)$$

where  $E_{q_s} = \hbar^2 q_s^2 / 2m^*$ ,  $E_{Q_s} = \hbar^2 Q_s^2 / 2m^*$  are the kinetic energies in a region with a characteristic size of respectively  $1/q_s$  and  $1/Q_s$ , and  $E_w = \hbar\omega$  is the harmonic oscillator energy.

And correspondingly the quantities

$$\beta^2 = \frac{1}{2\hbar^2} \frac{\xi'_s}{4\pi} \left\{ (e^{-z} - 1) \left[ \frac{1}{2sq_s} - \left( \frac{z}{sq_s} - 1 \right) \right] + 1 \right\} = \frac{1}{2\hbar^2} \frac{\xi''_s}{2\pi} \left\{ (1 - 2sQ_s u) e^z - 2z \left( w + \frac{z}{(2sQ_s)^2} \right) \right\}, \quad q = \frac{(\frac{1}{2}E_w + E_0 - E)}{\hbar}, \quad (35)$$

where a new quantity  $\xi'_s$ , having the same dimension (energy square) has been introduced in the first case according to

$$\xi'_s = \frac{\xi'_s}{sq_s} = \frac{n_I d a^2}{sq_s} \left( \frac{Ze^2}{8\pi\epsilon_0\epsilon_s a} \right)^2. \quad (36)$$

Using the newly introduced quantities, and performing the integration over  $t$  in Eq. (30) (using the general formula given in Ref. 14), the DOS can be rewritten as

$$\rho_1(E) = \frac{1}{2\pi\hbar} \left( \frac{m^*}{2\pi\hbar} \right) \omega^2 \frac{\sqrt{\pi}}{2} \beta^{-2} e^{-q^2/8\beta^2} D_1 \left( \frac{q}{\beta\sqrt{2}} \right). \quad (37)$$

Since we are interested in the DOS deep in the band tail, which can be reached by letting  $E \rightarrow -\infty$  ( $q \rightarrow \infty$ ) and using the asymptotic expansion of the parabolic cylinder function  $D_1(x)$  for large argument values namely,  $D_p(x) \sim e^{-x^2/2} x^p$ , we obtain the following expression for the low-energy DOS:

$$\rho_1(E) = \frac{1}{2\pi\hbar} \left( \frac{m^*}{2\pi\hbar} \right) \omega^2 \frac{\sqrt{\pi}}{2} \frac{q}{\beta^3} e^{-q^2/4\beta^2}. \quad (38)$$

Defining dimensionless energy for each of the cases considered,

$$\nu = \begin{cases} \frac{E_0 - E}{E_{q_s}}, & sq_s \gg 1, \quad aq_s \ll 1 \\ \frac{E_0 - E}{E_{Q_s}}, & sq_s \gg 1, \quad aq_s \gg 1 \end{cases} \quad (39)$$

we finally obtain for the deep band-tail DOS the following expressions, corresponding to the two cases:

$$\rho_1(\nu) = \frac{(E_{q_s} q_s)^2}{\xi_{q_s}^{(3/2)}} a(\nu, z) e^{-b(\nu, z)(E_{q_s}^2/2\xi_{q_s}')} \\ = \frac{(E_{Q_s} Q_s)^2}{\xi_{Q_s}^{(3/2)}} a(\nu, z) e^{-b(\nu, z)(E_{Q_s}^2/2\xi_{Q_s}')} \quad (40)$$

where the introduced dimensionless function  $a(\nu, z)$  and  $b(\nu, z)$  are given correspondingly by

$$a(\nu, z) = \begin{cases} \frac{(9\sqrt{2}/4z^2)(3/4z + \nu)}{\{(e^{-z} - 1)[1/2sq_s - (z/sq_s - 1)] + 1\}^{3/2}}, & sq_s \gg 1, \quad aq_s \ll 1 \\ \frac{(9/8z^2)(3/4z + \nu)}{\{(1 - 2sQ_s u)e^z - 2z(w + z/(2sQ_s)^2)\}^{3/2}}, & sq_s \gg 1, \quad aq_s \gg 1 \end{cases} \quad (41)$$

$$b(\nu, z) = \begin{cases} \frac{\pi(3/4z + \nu)^2}{(e^{-z} - 1)[1/2sq_s - (z/sq_s - 1)] + 1}, & sq_s \gg 1, \quad aq_s \ll 1 \\ \frac{2\pi(3/4z + \nu)^2}{(1 - 2sQ_s u)e^z - 2z(w + z/(2sQ_s)^2)}, & sq_s \gg 1, \quad aq_s \gg 1. \end{cases} \quad (42)$$

In order to determine the variational parameter  $\omega$  introduced in the trial action we shall choose  $z$  so as to minimize the argument of the exponential in the DOS or equivalently to maximize  $\rho_1(E)$ .<sup>15,16</sup> The best choice of  $z$  is found to satisfy the following transcendental equations, respective to the first and the second case:

$$6 - 6e^z + 3(6e^z - 7)z + 2(3 - 6\nu + 4e^z\nu)z^2 + 8\nu z^3 - 2sq_s(4\nu z^2 + 3z - 6) = 0, \quad (43)$$

$$-3e^z + \frac{3}{2}(e^z + 2w)z + 2\nu(e^z - 2w)z^2 - \frac{2\nu z^3}{(sQ_s)^2} - e^z sQ_s u(4\nu z^2 + 3z - 6) = 0. \quad (44)$$

The complete determination of the band-tail DOS requires the solution of these equations that can be performed only numerically. In the following section we obtain analytical asymptotic expressions for the dimensionless functions  $a(\nu)$  and  $b(\nu)$  in the two limiting cases of weak and strong screening and we shall calculate the DOS numerically for the general case.

### III. STUDY OF THE LIMITING CASES OF WEAK AND STRONG SCREENING

We obtain (see Appendix A) the following energy dependence for the dimensionless functions corresponding to the first case Eq. (43) in the weak screening limit  $\nu \gg 1$ :

$$a(\nu) \approx \frac{9\nu}{2^{3/2}(sq_s)^2}, \quad (45)$$

$$b(\nu) \approx \pi\nu^2$$

and correspondingly, in the strong screening limit  $\nu \ll 1$ ,

$$a(\nu) \approx a'_1 + a'_2\nu, \quad (46)$$

$$b(\nu) \approx b'_1 + b'_2\nu,$$

where  $a'_1, b'_1, a'_2, b'_2$  depend on the parameter  $sq_s$  and are given by (A7).

The weak screening result for the dimensionless functions corresponding to the second case Eq. (44) is

$$a(\nu) \approx \frac{9}{2^3(sQ_s)^4} \nu, \quad (47)$$

$$b(\nu) \approx 2\pi\nu^2$$

and in the strong screening limit we get

$$a(\nu) \approx a''_1 + a''_2\nu, \quad (48)$$

$$b(\nu) \approx b''_1 + b''_2\nu,$$

where  $a''_1, b''_1, a''_2, b''_2$  depend on the parameter  $sQ_s$  and are given by (A15).

From Eqs. (46) and (48) in the strong screening limit, it can be seen that if the energy is very small ( $\nu \rightarrow 0$ ) the dimensionless functions  $a(\nu)$  and  $b(\nu)$  tend to assume constant values. In the weak screening case the dependence of  $a(\nu)$ , as a function of the dimensionless energy, is linear and the  $b(\nu)$  dependence is quadratic for both limiting cases considered [see Eqs. (45) and (47)].

TABLE I. Power-law dependence of the dimensionless functions  $a(\nu)$  and  $b(\nu)$  on the dimensionless energy  $\nu$  for a Gaussian random potential for different dimensionality of the system ( $d$  representing the number of dimensions of the system) in the strong and weak screening limit.

| $d$ | $b(\nu)$                                                 | $a(\nu)$                               | $b(\nu)$                                          | $a(\nu)$                           |
|-----|----------------------------------------------------------|----------------------------------------|---------------------------------------------------|------------------------------------|
|     | strong screening $q = 1/L \rightarrow \infty, \nu \ll 1$ |                                        | weak screening $q = 1/L \rightarrow 0, \nu \gg 1$ |                                    |
| 1   | $\sqrt{3}\nu^{3/2}$                                      | $\frac{2^{3/2}}{\pi\sqrt{3}}\nu^{1/2}$ | $\nu^2$                                           | $\frac{1}{\pi\sqrt{2}}\nu$         |
| 2   | $2\nu$                                                   | $\frac{2^{5/2}}{\pi^{3/2}}\nu$         | $\nu^2$                                           | $\frac{1}{\pi^{3/2}\sqrt{2}}\nu^2$ |
| 3   | $\nu^{1/2}$                                              | $\frac{2^{11/2}}{\pi^2}\nu^{3/2}$      | $\nu^2$                                           | $\frac{1}{\pi^2\sqrt{2}}\nu^3$     |

The behavior of  $a(\nu)$  and  $b(\nu)$  in the general case of a  $d$ -dimensional system has been studied by Sa-yakanit<sup>17</sup> and expressions for both dimensionless functions of the DOS have been obtained in the case of a Gaussian autocorrelation function. According to Ref. 17, we can construct the following Table I summarizing the power-law dependence of the above dimensionless functions on the dimensionality of the system (for a Gaussian potential).

On the other hand we have presented our results and the results for the case of a 3D Coulomb potential as a model random impurity potential according to Ref. 9 in Table II.

Let us consider first the weak screening limit. As can be seen from Table I and Table II, the exponent  $b(\nu)$  in the weak screening limit is proportional to  $\nu^2$  independent of the system dimension, while the dimensionless function in the preexponential factor  $a(\nu)$  depends on the number of dimensions. In both the limiting cases considered, the dependence of  $a(\nu)$  as a function of  $\nu$  is linear, while for the 3D Gaussian potential it is cubic and for the 3D-screened Coulomb

potential the power of the dependence is  $7/2=3.5$ , and for the 2D case of a random Gaussian potential it is quadratic. It is well known that the preexponential factor strongly depends on the potential shape, thus leading to different power laws. As the random potential of the problem considered represents a solution of Poisson's equation, including the 2D electron gas screening within the 2D Thomas-Fermi model, which differs from both the pure screened Coulomb potentials and Gaussian potential, we can expect the observed difference. On the other hand, the problem turns out to be quasi-2D instead of 3D, which also leads to the difference between the 2D case of a Gaussian potential (see Table I;  $d=2$ ) and our weak screening results (Table II). Now, let us consider the strong screening limit. The behavior of  $b(\nu)$  observed (Table II) is linear exactly as in the 2D case of a Gaussian potential (Table I). The behavior of the preexponent  $a(\nu)$  is also the same as in the 2D Gaussian potential case. Thus our problem in the strong screening limit approaches the two-dimensional Gaussian potential case,

TABLE II. Comparison between the power-law dependences of the dimensionless functions  $a(\nu)$  and  $b(\nu)$  on the dimensionless energy  $\nu$  for the 3D screened Coulomb random potential and the potential, representing a solution of Poisson's equation for the quasi-3D problem considered in the two limiting cases of the general correlation function. The results are presented for the weak screening and strong screening limit.

| $d$              |              | $b(\nu)$                                           | $a(\nu)$                         | $b(\nu)$                                    | $a(\nu)$                           |
|------------------|--------------|----------------------------------------------------|----------------------------------|---------------------------------------------|------------------------------------|
|                  |              | strong screening $q \rightarrow \infty, \nu \ll 1$ |                                  | weak screening $q \rightarrow 0, \nu \gg 1$ |                                    |
| 3D               |              | $2\sqrt{\pi}\nu^{1/2}$                             | $\frac{1}{\pi\sqrt{2}}\nu^{3/2}$ | $\nu^2$                                     | $\frac{\sqrt{2}}{9\pi^3}\nu^{7/2}$ |
| Screened Coulomb |              |                                                    |                                  |                                             |                                    |
| Quasi-3D         | case 1:      | $b'_1 + b'_2\nu$                                   | $a'_1 + a'_2\nu$                 | $\pi\nu^2$                                  | $\frac{9\nu}{2^{3/2}(sq_s)^2}$     |
|                  | $sq_s \gg 1$ |                                                    |                                  |                                             |                                    |
|                  | $aq_s \ll 1$ |                                                    |                                  |                                             |                                    |
| Quasi-3D         | case 2:      | $b''_1 + b''_2\nu$                                 | $a''_1 + a''_2\nu$               | $2\pi\nu^2$                                 | $\frac{9}{2^3(sq_s)^4}\nu$         |
|                  | $sq_s \gg 1$ |                                                    |                                  |                                             |                                    |
|                  | $aq_s \gg 1$ |                                                    |                                  |                                             |                                    |

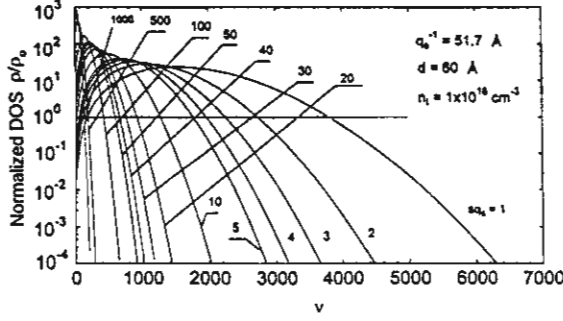


FIG. 2. Normalized 2D DOS in the band tail at the interface of a single GaAs-Al<sub>x</sub>Ga<sub>1-x</sub>As heterojunction as a function of the dimensionless energy  $v$  for different values of the parameter  $sq_s$ , where  $q_s^{-1} = 51.7 \text{ Å}$ , 3D doping impurity concentration  $n_i = 1 \times 10^{18} \text{ cm}^{-3}$  and doping layer width  $d = 60 \text{ Å}$ .

while in the weak screening limit it is similar to the 1D Gaussian potential case. This reflects the quasi-two-dimensionality of our problem.

#### IV. NUMERICAL RESULTS

In this section we present numerical calculations for the band-tail DOS in GaAs-Al<sub>x</sub>Ga<sub>1-x</sub>As single heterostructures. The dielectric constants and effective masses are assumed to be equal in both materials, namely,  $\epsilon_s = 13.1$  and  $m^* = m_z = 0.067m_0$ . The unit length of the system is the effective Bohr radius, which is evaluated to be  $a_B^* = 4\pi\epsilon_0\epsilon_s\hbar^2/m^*e^2 \approx 103 \text{ Å}$  and the energy unit is the effective Rydberg:  $Ry^* = m^*e^4/2(4\pi\epsilon_0\epsilon_s)^2\hbar^2 \approx 5.3 \text{ meV}$ . The DOS is normalized with respect to the free-electron DOS for the lowest conduction subband, and in real units is equal to:  $\rho_0 \approx 2.799 \times 10^{10} \text{ meV}^{-1} \text{ cm}^{-2}$ . We have calculated the band-tail DOS of a heterostructure for different values of the characteristic parameters as a 3D-impurity concentration  $n_i$ , spacer layer thickness  $s$ , doping layer thickness  $d$ , and 2D EG thickness  $a$ . The 2D EG inverse screening length  $q_s$  is the same as the one discussed by Ando *et al.*<sup>8</sup> and is given by

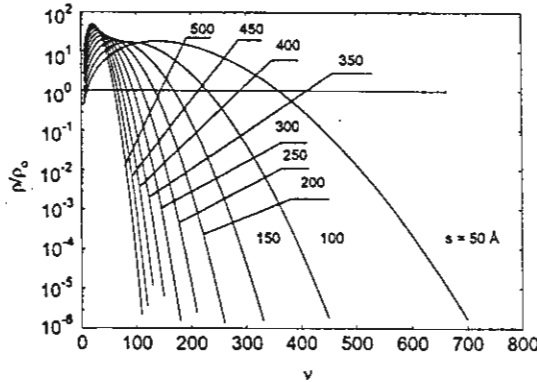


FIG. 3. Normalized 2D DOS in the band tail at the interface of a single GaAs-Al<sub>x</sub>Ga<sub>1-x</sub>As heterojunction vs dimensionless energy  $v$  as a function of  $s$  (spacer layer thickness) in Å for  $q_s^{-1} = 51.7 \text{ Å}$ , 3D doping impurity concentration  $n_i = 1 \times 10^{18} \text{ cm}^{-3}$ , doping layer width  $d = 50 \text{ Å}$  and 2D EG thickness  $a = 100 \text{ Å}$ .

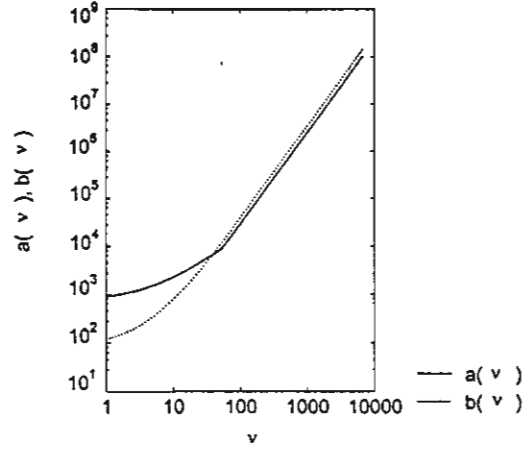


FIG. 4. Plot of prefactor  $a(v)$  and the exponent  $b(v)$  in the band-tail DOS with respect to the dimensionless energy  $v$ .

$q_s = 2g_v/a_B^*$ , where  $g_v$  is a valley degeneracy factor, giving the number of the equivalent energy bands, which we assume equals 1 for GaAs and Al<sub>x</sub>Ga<sub>1-x</sub>As. The screening length calculated using the above constants is equal to  $q_s^{-1} \approx 51.7 \text{ Å}$ .

#### Band-tail DOS calculations

The DOS in the band tail at the interface of a single GaAs-Al<sub>x</sub>Ga<sub>1-x</sub>As heterojunction normalized to the free-electron 2D-DOS has been computed using expression (40) for the DOS derived in the Sec. II. For the first case ( $sq_s \gg 1, aq_s \ll 1$ ) the normalized band-tail results are presented in Fig. 2 for different values of the dimensionless parameter  $sq_s$ . The numerically calculated normalized band-tail DOS in the second case, i.e.,  $sq_s \gg 1$  and  $aq_s \gg 1$  corresponding to finite thickness of the 2D EG is presented in Fig. 3.

It should be noted that only the DOS deep in the band tail below unity has a physical meaning (similar to the method of Halperin and Lax<sup>16</sup>). As for small energies (near to the conduction-band edge) the path-integral results for the DOS lead to an unphysical initial region of the curve. As can be

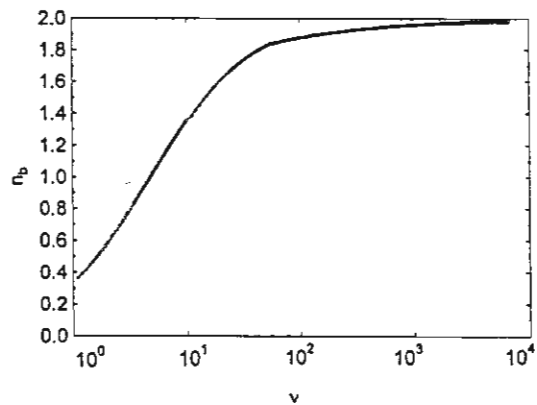


FIG. 5. Plot of logarithmic derivative  $n_b(v) = d \ln[b(v)]/d \ln v$  of the exponent  $b(v)$  in the band-tail DOS as a function of the dimensionless energy  $v$ . The function is smoothly varying in the selected energy interval from a value close to 0.4 up to 2.

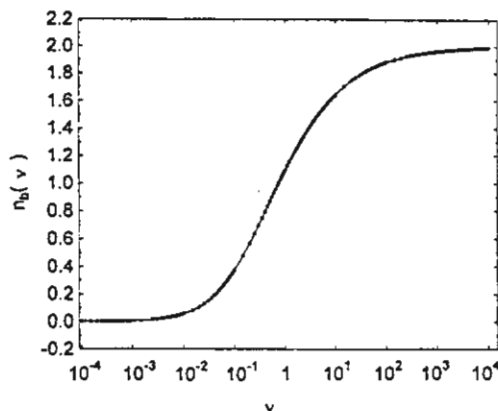


FIG. 6. Plot of the logarithmic derivative of  $b(\nu)$  obtained analytically from Eq. (49), using numerically calculated values of  $z_{\min}$  as a function of the dimensionless energy  $\nu$ .

seen from Fig. 2 and Fig. 3, the extent of the band tail in the 2D DOS tail in the forbidden gap is monotonously reduced with increasing spacer layer thickness  $s$ . This is in agreement with the experimentally observable reduced influence of the random potential fluctuations on the 2D EG with increasing thickness of the undoped spacer layer, thus enhancing the electron mobility.

The dimensionless functions  $a(\nu)$  and  $b(\nu)$  corresponding to the first correlator are plotted against the dimensionless energy  $\nu$  for  $s q_s = 10$  (Fig. 4).

It is reasonable to assume a power-law dependence on the dimensionless energy for the exponent  $b(\nu)$  (see Table II), namely,  $b(\nu) = c_b \nu^{n_b}$ . In order to obtain the power of the energy dependence of the band-tail DOS we calculate the logarithmic derivative  $n_b(\nu) = d \ln[b(\nu)] / d \ln \nu$ . The logarithmic derivative of the exponent  $b(\nu)$  is calculated numerically for the above case and is plotted in Fig. 5 against the dimensionless energy  $\nu$ .

It should be noted that for  $\nu < 1$  the exponent  $b(\nu)$  has no minimum for the chosen set of parameters.

The same quantity has been calculated by taking analytically the derivative of the logarithms of Eq. (42) with respect

to  $\ln \nu$ , taking at each energy  $\nu$  the minimum value of  $z$  corresponding to it. Thus we obtain the following simple relation:

$$n_b(\nu) = \frac{2\nu}{3/4z_{\min}^2 + \nu}, \quad (49)$$

which is plotted in Fig. 6 versus the dimensionless energy.

It can be seen (from both Fig. 5 and Fig. 6) that in the weak screening case ( $\nu \gg 1$ ) the power law of the exponent in the DOS is quadratic, while in the strong screening limit ( $\nu \ll 1$ ) it approaches zero, which means that there is no energy dependence for very small energies and the DOS becomes a constant. This is in agreement with the analytical results quoted in Table II.

We have investigated numerically the behavior of the tail in the DOS corresponding to the second case of a finite 2D EG thickness, by varying the important physical parameters of the system. In Fig. 7 the 3D plot of the normalized band-tail DOS as a function of the spacer layer thickness with the 2D EG width  $a$  as parameter is given.

In all of the cases considered, the extent of the tail in the DOS monotonously decreases with increasing spacer layer thickness  $s$ . It can be seen that the extent of the band tail in the gap increases as the 2D EG width  $a$  increases at a given value of spacer layer thickness. This can be easily demonstrated by plotting the normalized band-tail DOS as a function of the 2D EG width  $a$  (Fig. 8).

The increase of the band tail in the DOS with increasing 2D EG width can be explained by the change of the character of the screening during the transition from quasi-2D to quasi-3D. According to Eq. (5), the 3D inverse screening length  $Q_s$  is inversely proportional to the 2D EG width  $a$  (at a fixed 2D EG screening length  $q_s^{-1}$ ). Therefore by increasing  $a$  the screening of the random potential fluctuations will decrease thus leading to an extension of the band tail in the gap.

Let us consider now the dependence of the band-tail DOS on the doped region width  $d$ . In Fig. 9 the plot of the normalized band-tail DOS at the interface is presented as a function of  $d$ .

Since the impurity concentration is kept constant, the observed increase of the extent of the band tail with increasing

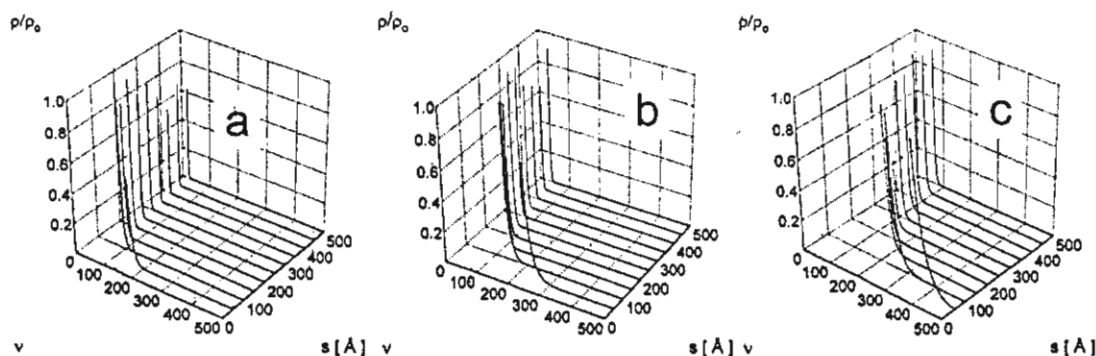


FIG. 7. 3D plot of the normalized band-tail DOS vs dimensionless energy  $\nu$  and  $s$  (spacer layer thickness) at the interface of a single GaAs- $\text{Al}_x\text{Ga}_{1-x}\text{As}$  heterojunction calculated using the following parameters: 2D EG screening length  $q_s^{-1} = 51.7 \text{ \AA}$ , doping region width  $d = 50 \text{ \AA}$ , 3D doping impurity concentration  $n_I = 1 \times 10^{18} \text{ cm}^{-3}$  at 3 different widths  $a$  of the 2D EG (a)  $a = 30 \text{ \AA}$ ; (b)  $a = 50 \text{ \AA}$ ; (c)  $a = 100 \text{ \AA}$ .

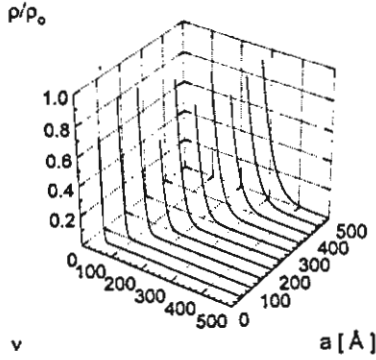


FIG. 8. 3D plot of the normalized band-tail DOS vs dimensionless energy  $\nu$  and  $a$  (2D EG width) at the interface of a single GaAs-Al<sub>x</sub>Ga<sub>1-x</sub>As heterojunction calculated using the following parameters: 2D EG screening length  $q_s^{-1} = 51.7$  Å, doping region width  $d = 50$  Å, 3D doping impurity concentration  $n_i = 1 \times 10^{18}$  cm<sup>-3</sup> and spacer layer thickness  $s = 450$  Å.

doped region thickness is due to the increased total number of impurities in the doped region with increased volume (in order to keep constant  $n_i$ ). This in turn leads to greater fluctuations and therefore a longer band tail in the gap at the interface.

Finally, let us consider the dependence of the band-tail DOS on the impurity centers concentration presented in Fig. 10. The observed increase of the extent of the tail in the band gap is due to the increased number of impurity centers in the highly doped barrier layer resulting in greater fluctuations.

In order to compare the results for the band-tail DOS obtained in the two limiting cases of the 2D correlation function, we need to represent the expressions in Eq. (40) in the same units (see Appendix B). Thus we get the band-tail DOS in the same units:

$$\frac{\rho_1^{(1)}(\nu)}{Q_s^2/E_Q \xi_2^{3/2}} = \left( \frac{s a q_s^2}{16 \xi_1} \right)^{3/2} a(\nu, z) \exp \left( - \frac{b(\nu, z) s a q_s^2}{16 \xi_2} \right), \quad (50)$$

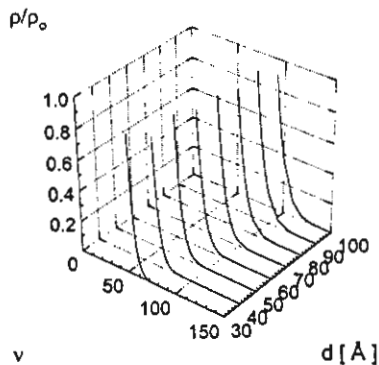


FIG. 9. 3D plot of the normalized band-tail DOS vs dimensionless energy  $\nu$  and  $d$  (doping region thickness) at the interface of a single GaAs-Al<sub>x</sub>Ga<sub>1-x</sub>As heterojunction at  $a = 100$  Å,  $s = 450$  Å,  $q_s^{-1} = 51.7$  Å and  $n_i = 1 \times 10^{18}$  cm<sup>-3</sup>.

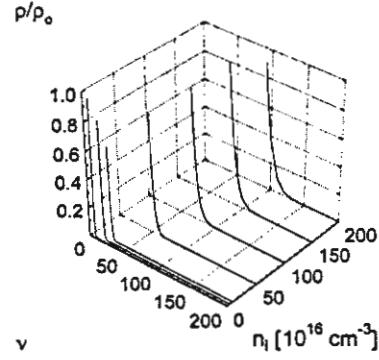


FIG. 10. 3D plot of the normalized band-tail DOS vs dimensionless energy  $\nu$  for different impurity densities  $n_i$  at the interface of a single GaAs-Al<sub>x</sub>Ga<sub>1-x</sub>As heterojunction at  $a = 100$  Å,  $s = 450$  Å,  $q_s^{-1} = 51.7$  Å, and  $d = 50$  Å.

$$\frac{\rho_1^{(2)}(\nu)}{Q_s^2/E_Q \xi_2^{3/2}} = a(\nu, z) \exp \left( - \frac{b(\nu, z)}{2 \xi_2} \right). \quad (51)$$

Equation (50) together with Eq. (51) determine the band-tail DOS depending on the following parameters:  $\xi_2$ ,  $s q_s$ , and  $a q_s$ . We have plotted the normalized DOS as a function of the dimensionless energy in both cases for four values of the dispersion of the random potential energy  $\xi_2$  hereafter referred to as  $\xi$  and keeping constant the rest of the parameters ( $s q_s$  and  $a q_s$ ) in Fig. 11.

As can be seen from Fig. 11, the extent of the band tail increases monotonously in both cases while increasing the disorder parameter  $\xi$ . It should be noted that the DOS band tail is more sensitive to a change in  $\xi$  in the first case as compared to the second case.

The results of calculating the band-tail DOS as a function of the parameter  $s q_s$  while the disorder parameter  $\xi$  and the  $a q_s$  parameter are fixed, are shown in Fig. 12.

For both cases the extent of the band-tail DOS decreases with increasing spacer layer thickness  $s$ , which is in agreement with the experimental observations. The DOS corresponding to the first case is more sensitive to the variation of  $s$  than the DOS corresponding to the second case. Therefore the in-plane potential fluctuations are strongly affected by the spacer layer thickness and result in a deeper band tail at the interface.

Finally, we shall study the dependence of the band-tail DOS on the parameter  $a q_s$  (i.e., on the width  $a$  of the 2D EG in the inversion layer). The DOS results are shown in Fig. 13 for four values of the parameter  $a q_s$ .

It is clearly seen from Fig. 13 that with the increasing of the inversion layer width  $a$  the curves corresponding to the two expressions for the band-tail DOS tend toward each other and for very large values of  $a$  we can expect that they will coincide. At a very large inversion layer thickness  $a$  the well material can be regarded as a metal plate of a capacitor and therefore the result for the 2D DOS should coincide with that obtained by using the  $a$ -independent correlator.

## V. SEMICLASSICAL LIMIT OF THE DOS

As pointed out in Ref. 10, the semiclassical approach is the only existing closed analytical formula that covers the

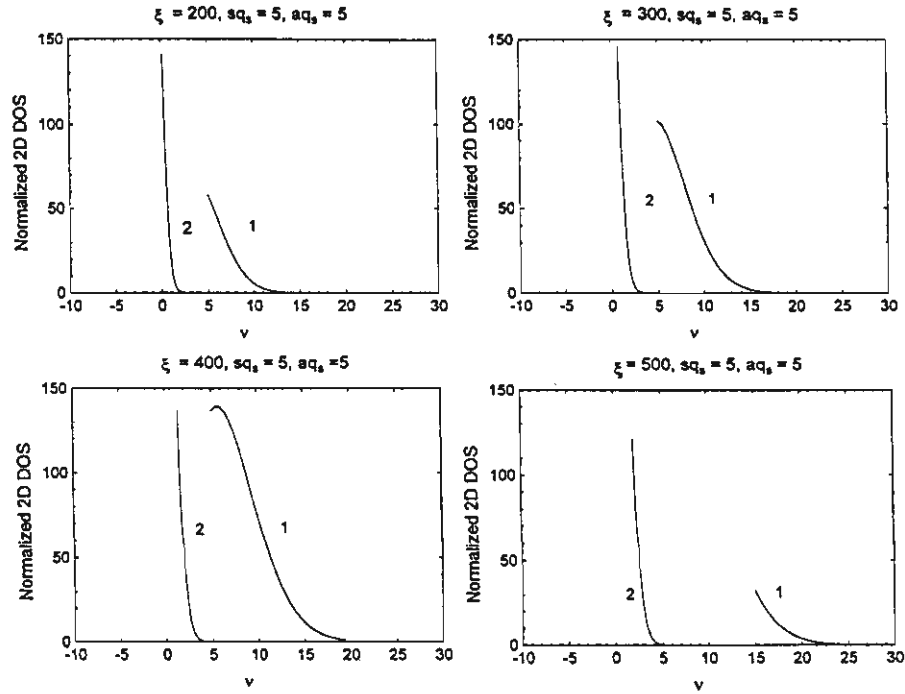


FIG. 11. Plot of the band-tail DOS in units of  $Q_s^2/(E_Q \xi^{3/2})$  vs dimensionless energy  $v$  with the dispersion of the random potential energy  $\xi = 200, 300, 400$ , and  $500$  as a parameter ( $sq_s = aq_s = \text{const} = 5$ ); case 1:  $sq_s \gg 1$ ,  $aq_s \ll 1$ ; case 2:  $sq_s \gg 1$ ,  $aq_s \gg 1$ .

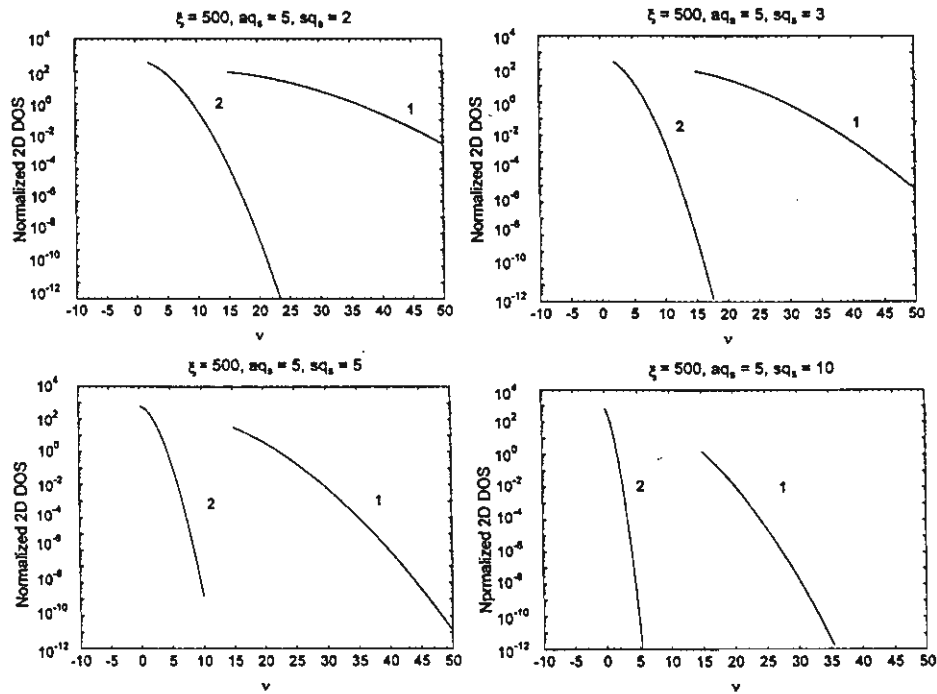


FIG. 12. Semilogarithmic plot of the band-tail DOS in units of  $Q_s^2/(E_Q \xi^{3/2})$  vs dimensionless energy  $v$  with  $sq_s = 2, 3, 5, 10$  as a parameter; the dispersion of the random potential energy  $\xi = 500$ ,  $aq_s = 5$  have been kept constant; case 1:  $sq_s \gg 1$ ,  $aq_s \ll 1$ ; case 2:  $sq_s \gg 1$ ,  $aq_s \gg 1$ .

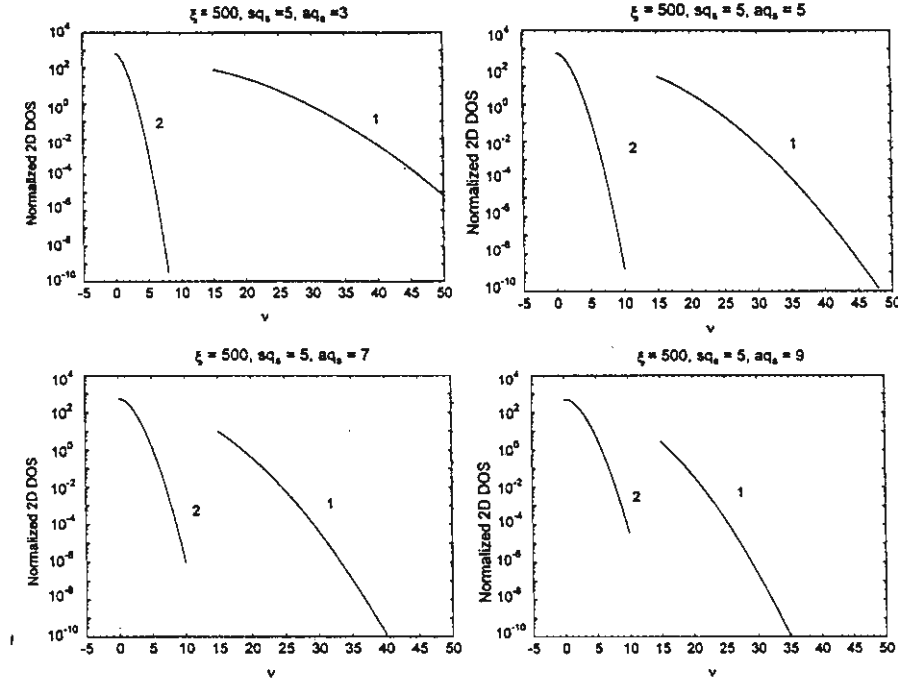


FIG. 13. Semilogarithmic plot of the band-tail DOS in units of  $Q_s^2/(E_0 \xi^{3/2})$  vs dimensionless energy  $v$  with  $aq_s = 3, 5, 7, 9$  as a variation parameter ( $\xi = 500, sq_s = 5$ ); case 1:  $sq_s \gg 1, aq_s \ll 1$ ; case 2:  $sq_s \gg 1, aq_s \gg 1$ .

whole energy range. However, it ceases to be valid in the deep energy tail region and is not capable of describing the impurity bands. In order to compare our results for the band-tail DOS we need to obtain the semiclassical DOS at high energies. Since the general path-integral expression (23) for the DOS is valid in the whole energy interval, in order to obtain the Kane semiclassical DOS evaluating the contribution of only the high energy states it is necessary to take the limit as  $t \rightarrow 0$  of Eq. (23) instead of taking the low-energy

limit as  $t \rightarrow \infty$ , as in the case of a deep energy band-tail DOS Eq. (27). This limiting procedure has a simple physical meaning if we think of it in terms of the Heisenberg uncertainty principle for the energy and time,  $Et \gg \hbar$ .

Let us concentrate now on the derivation of the semiclassical approximation for the DOS. Consider the general expression (23). The limit  $t \rightarrow 0$  leads to a very much simplified expression for the DOS in both the first and second cases:

$$\begin{aligned} \rho_1^{sc}(E) &= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \left( \frac{m^*}{2\pi i \hbar t} \right) \exp \left[ -\frac{i}{\hbar} (E_0 - E)t - \frac{1}{2\hbar^2} \frac{\xi_{q_s}'}{4\pi} t^2 \right] \\ &= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \left( \frac{m^*}{2\pi i \hbar t} \right) \exp \left[ -\frac{i}{\hbar} (E_0 - E)t - \frac{1}{2\hbar^2} \frac{\xi_{q_s}''}{2\pi} t^2 (1 - 2Q_s u) \right]. \end{aligned} \quad (52)$$

The time integration can be performed using the generalization of the formula given in Ref. 14, which leads to a parabolic cylinder function of order  $-1$ :

$$\rho_1^{sc}(E) = \frac{m^*}{(2\pi)^{3/2} \hbar^2} e^{-(E_0 - E)\pi/\xi_{q_s}'} D_{-1} \left( \frac{(E_0 - E)\sqrt{4\pi}}{\sqrt{\xi_{q_s}'}} \right) = \frac{m^*}{(2\pi)^{3/2} \hbar^2} e^{-(E_0 - E)^2 \pi/2(1 - 2Q_s u)\xi_{q_s}''} D_{-1} \left( \frac{(E_0 - E)\sqrt{2\pi}}{\sqrt{\xi_{q_s}''(1 - 2suQ_s)}} \right). \quad (53)$$

Let us define the following parameters:

$$\xi_{q_s} = \frac{\xi'_{q_s}}{4\pi} \quad (54)$$

and

$$\xi_{Q_s} = \frac{\xi''_{Q_s}(1-2suQ_s)}{2\pi} \quad (55)$$

and multiply the DOS by a factor of 2 in order to account for the spin degeneracy of each energy level. Equation (53) can be thus rewritten as

$$\rho_1^{sc}(E) = \begin{cases} \frac{2m^*}{(2\pi)^{3/2}\hbar^2} e^{-(E_0-E)^2/4\xi_{q_s}} D_{-1}\left(\frac{(E_0-E)}{\sqrt{\xi_{q_s}}}\right) \\ \frac{2m^*}{(2\pi)^{3/2}\hbar^2} e^{-(E_0-E)^2/4\xi_{Q_s}} D_{-1}\left(\frac{(E_0-E)}{\sqrt{\xi_{Q_s}}}\right) \end{cases} \quad (56)$$

In order to obtain the DOS in the low-energy tail we shall take the limit  $|E-E_0| \rightarrow \infty$  for negative energies  $E - E_0/\sqrt{\xi_{q_s}} \ll -1$  ( $E - E_0/\sqrt{\xi_{Q_s}} \ll -1$ ). Using the asymptotic representation of the parabolic cylinder function for large argument values (see, for example, Ref. 18):  $D_{-1}(x) \sim e^{x^2/4}/x$  we get that

$$\begin{aligned} \rho_1^{sc}(E) &= \frac{m^*}{\pi^{3/2}\hbar^2\sqrt{2}} \frac{\sqrt{\xi_{q_s}}}{(E_0-E)} e^{-(E_0-E)^2/2\xi_{q_s}} \\ &= \frac{m^*}{\pi^{3/2}\hbar^2\sqrt{2}} \frac{\sqrt{\xi_{Q_s}}}{(E_0-E)} e^{-(E_0-E)^2/2\xi_{Q_s}} \end{aligned} \quad (57)$$

Equation (56) represents the semiclassical Kane result for the DOS in the band tail. Let us consider the other limiting case for positive  $E-E_0$ . Using the expansion of the parabolic cylinder function of a large negative argument (see Ref. 18, pp. 687 and 689) we get the following expressions for the 2D free-electron DOS in terms of the error function:

$$\begin{aligned} \rho_1^{sc}(E) &= \frac{m^*}{2\pi\hbar^2} \left[ 1 + \operatorname{erf}\left(\frac{E-E_0}{\sqrt{\xi_{q_s}}}\right) \right] \\ &= \frac{m^*}{2\pi\hbar^2} \left[ 1 + \operatorname{erf}\left(\frac{E-E_0}{\sqrt{\xi_{Q_s}}}\right) \right] \end{aligned} \quad (58)$$

In order to compare our results for the band-tail DOS with the semiclassical limit we need to represent both expressions in the same units. From Appendix C for the band-tail DOS we obtain, respectively in the first and second cases,

$$\rho_1^{BT}(\nu) = a(\nu, z) e^{-b(\nu, z)/2\xi_1} = a(\nu, z) e^{-b(\nu, z)/2\xi_2} \quad (59)$$

Representing the semiclassical expression for the DOS in the same units we get

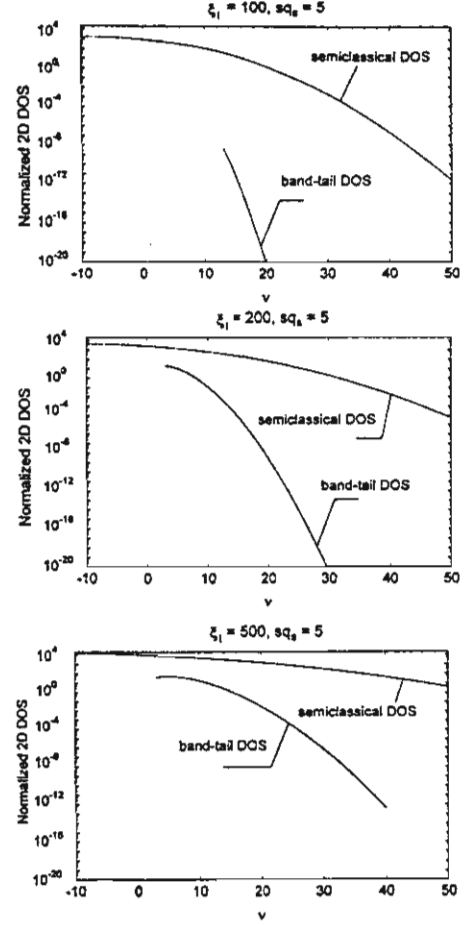


FIG. 14. Plot of the semiclassical 2D DOS and the band-tail 2D DOS in units of  $q_s^2/E_q \xi_1^{3/2}$  as a function of the dimensionless energy  $\nu$  for  $\xi_1 = 100, 200, 500$  and  $sq_s = 5$ .

$$\begin{aligned} \rho_1^{sc}(\nu) &= \left(\frac{\xi_1}{2\pi}\right)^{3/2} e^{-\nu^2\pi/\xi_1} D_{-1}\left(\frac{2\nu\sqrt{\pi}}{\sqrt{\xi_1}}\right) \\ &= \left(\frac{\xi_2}{2\pi}\right)^{3/2} e^{-\nu^2\pi/2\xi_2(1-2suQ_s)} D_{-1}\left(\frac{\nu\sqrt{2\pi}}{\sqrt{\xi_2(1-2suQ_s)}}\right) \end{aligned} \quad (60)$$

Therefore, the corresponding rows of Eqs. (59) and (60) depend on the same parameter set and can be compared. The results of the comparison between the semiclassical expression and the band-tail expression for the DOS in the first case in units of  $q_s^2/E_q \xi_1^{3/2}$  [first row of Eqs. (59) and (60)] for three different values of the disorder parameter  $\xi_1$  and fixing  $sq_s = 5$  are shown in Fig. 14. From Fig. 14 it can be seen that the extent of the band tail as well as the Kane tail increase as the dispersion of the random potential energy increases.

In Fig. 15 we have plotted both results for the semiclassical DOS and the band-tail corresponding to the first case at a fixed disorder parameter  $\xi_1$  while varying the spacer layer thickness (or equivalently the  $sq_s$  parameter).

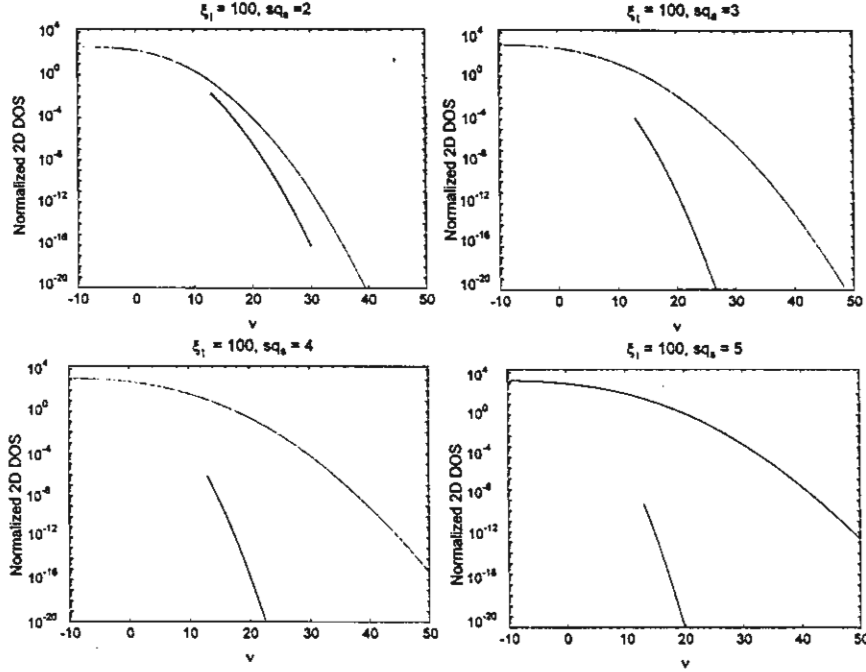


FIG. 15. Plot of the semiclassical 2D DOS (upper curve) and band-tail 2D DOS (lower curve) in units of  $q_s^2/E_Q \xi_1^{3/2}$  as a function of the dimensionless energy  $\nu$  at a fixed dispersion of the random potential energy  $\xi_1 = 100$  and  $sQ_s = 2, 3, 4, 5$ .

It is clearly seen that the extent of the low-energy band tail of the DOS in the band gap decreases, as the spacer layer thickness  $s$  increases. This can be attributed to the decay of the amplitude of the impurity potential fluctuations with increasing distance from the interface.

Similar to the first case, the DOS in units of  $Q_s^2/E_Q \xi_1^{3/2}$  is plotted against the dimensionless energy  $\nu$  in Fig. 16 for three different dispersions of the random potential energy while keeping constant the parameter  $sQ_s$ . Increasing the disorder parameter  $\xi_2$  the band tail extends more in the forbidden gap for both the semiclassical and low-energy DOS. Upon increasing the characteristic parameter  $sQ_s$  in the second case where we keep the disorder parameter  $\xi_2$  fixed, the tail in both cases shortens as expected (Fig. 17).

Generally the path-integral method yields the DOS in the whole energy range but only asymptotic expressions can be obtained for very high energies (near the band edge) and very low energies deep in the band tail. For intermediate energies no asymptotic expression has been obtained. Our aim is to study the behavior of both asymptotics for the DOS in the two-dimensional case.

## VI. COMPARISON WITH OTHER THEORETICAL APPROACHES FOR DOS CALCULATION IN 2D

In this section we discuss our results and compare them with other theoretical calculations of the 2D DOS.

### A. Generalized semiclassical approach and the path-integral method in 2D

The semiclassical method of calculating the DOS due to Kane<sup>19</sup> and Sklovskii and Efros<sup>20</sup> has been generalized by

Van Mighem *et al.*<sup>10</sup> The main assumption in the method is of smoothly varying random potential fluctuations within the electron wavelength, which is equivalent to considering only the electrons with energies sufficiently higher than the average potential energy such that the actual fluctuating potential can be replaced by the smoothed slowly varying potential. According to Ref. 10 this approximation applied to the non-interacting 2D Fermi gas leads to the following expression for the 2D DOS in the so-called high density limit (HDL) when the impurity concentration is very large ( $n_I \rightarrow \infty$ ):

$$\rho_{2n}(E) = \frac{m^*}{2\pi\hbar} \left[ 1 + \operatorname{erf} \left( \frac{E}{\sigma_{2n}\sqrt{2}} \right) \right], \quad (61)$$

where the subscript  $n$  stands for the noninteracting Fermi gas and the dispersion of the random potential is given by

$$\sigma_{2n} = \frac{e^2}{8\pi\epsilon_2 k_{2n}} \left( \frac{n_2}{\pi} \right)^{1/2}. \quad (62)$$

In the above expression  $\epsilon_2$  is the 2D dielectric constant and the zero temperature 2D inverse screening length is given by

$$k_{2n} = \left( \frac{m^* e^2}{4\pi^2 \hbar^2 \epsilon_2} \right)^{1/2}, \quad (63)$$

where  $n_2$  is the 2D impurity density and the energy zero has been chosen to coincide with the average potential energy ( $E_0 = 0$ ).

On the other hand, we have obtained the 2D free-electron DOS (58) as a limit of the general path-integral expression for the DOS, which gives exactly the same result [cf. Eqs.

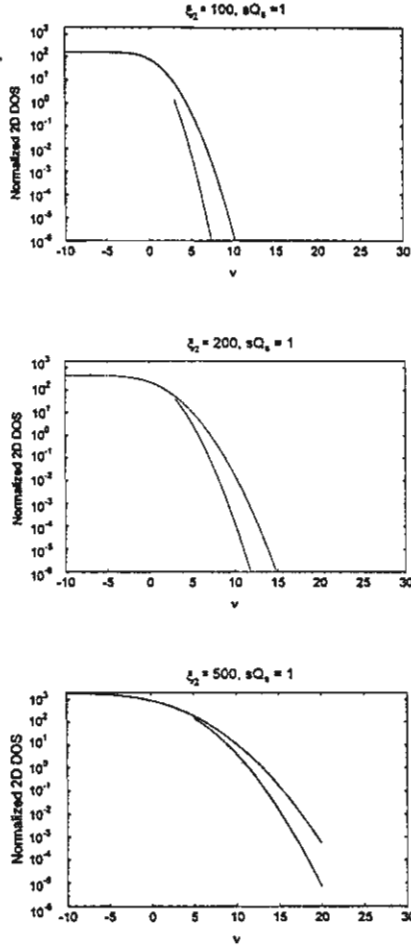


FIG. 16. Plot of the semiclassical (upper curve) and low-energy band tail results (lower curve) for the 2D DOS in the second case in units of  $Q_s^2/E_Q \xi_2^{3/2}$  as a function of the dimensionless energy  $\nu$  at  $sQ_s = 1$  for  $\xi_2 = 100, 200, 500$ .

(58) and (61)]. By comparing the arguments of Eq. (61) and the first and second case results for the DOS from Eq. (58) we can obtain a relationship between the dispersion of the random potential as defined by Van Mighem *et al.*,<sup>10</sup> and the dispersion of our problem, which is given by

$$\sigma_{2n}\sqrt{2} = \begin{cases} \frac{\sqrt{\xi'}}{2\sqrt{\pi s q_s}}, & s q_s \gg 1, \quad a q_s \ll 1 \\ \frac{\sqrt{\xi_Q(1-2suQ_s)}}{\sqrt{\pi}}, & s q_s \gg 1, \quad a q_s \gg 1. \end{cases} \quad (64)$$

Substituting the expressions for the dispersions from Eqs. (54) and (55) and subsequently from Eqs. (31) and (32) we get a simple relationship between the dielectric constants in 2D and 3D corresponding to the first and second cases under consideration:

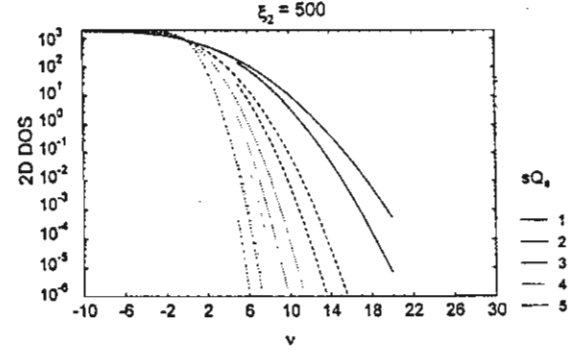


FIG. 17. Plot of the 2D DOS in the semiclassical limit (upper curve) and the low-energy band-tail DOS (lower curve) in units of  $Q_s^2/E_Q \xi_2^{3/2}$  vs dimensionless energy  $\nu$  at  $\xi_2 = 500$  for  $sQ_s = 1, 2, 3, 4, 5$ .

$$\varepsilon_2 = \begin{cases} 8\pi s q_s a_B^* \varepsilon_3 \\ 4\pi(aQ_s)^2 \\ 1 - 2suQ_s \end{cases} a_B^* \varepsilon_3. \quad (65)$$

Generally the characteristic length of the problem in the 2D case is the effective Bohr radius and we can expect that  $\varepsilon_2 = a_B^* \varepsilon_3$ ; the multipliers depend on the geometry of the system for the particular problem considered.

In order to compare our low-energy band-tail results for the 2D DOS it is necessary to represent both expressions as a function of the same argument. Using Appendix D we get the following expression in the band tail:

$$\left(\frac{\pi \hbar^2}{m^*}\right) \rho_1(\eta^*) = \left(\frac{2^{5/2} \pi}{4^3}\right) \eta^{*3} a(\eta^*, z) e^{-b(\eta^*, z) 16 \eta^{*2}} \quad (66)$$

and the normalized 2D semiclassical expression is correspondingly:

$$\left(\frac{\pi \hbar^2}{m^*}\right) \rho_{2n}(\eta^*) = \frac{1}{2} [1 + \text{erf}(\eta^*)]. \quad (67)$$

Since the dimensionless functions  $a(\nu, z)$  and  $b(\nu, z)$  depend in the first case on the parameter  $s q_s$ , we can compare Eqs. (66) with (67) for different parameter values, thus obtaining a family of curves. In Fig. 18 the semiclassical 2D DOS and our results corresponding to the first case are plotted on the same graph:

As can be seen from Fig. 18, an asymmetry of the step occurs around  $E^* = 0$  if the band-tail DOS is taken into account. This asymmetry has been experimentally observed in the optical absorption data of doped quantum wells.<sup>21</sup>

#### B. Multiple scattering method and the path-integral method in 2D

We have compared our results for the semiclassical and band-tail DOS with the calculations of the 2D DOS using the multiple-scattering theory method<sup>11</sup> applied to heterostructures. The multiple-scattering method accounts for the electron-impurity interaction at all orders in the electron-impurity potential and at all orders of the impurity concen-

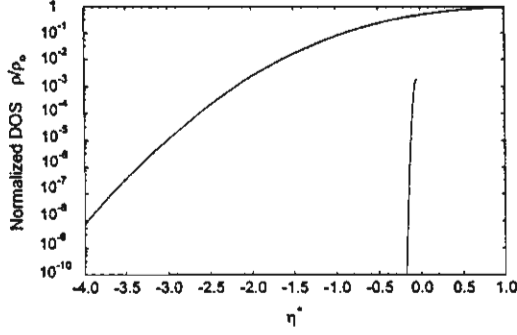


FIG. 18. Plot of the semiclassical (upper curve) and low-energy band-tail 2D DOS (lower curve) normalized with respect to the free-electron density as a function of the dimensionless parameter  $\eta^* = \eta(\pi s/q, a^2)^{1/2}$ . The 2D band-tail DOS is calculated for  $s q_s = 1$  using the expression (66) corresponding to the first case.

tration. Many body effects (screening and exchange-correlation energy) have been included in the self-energy of Ref. 11. Comparison is performed for the case where the charged impurity centers are located in the barrier material ( $\text{Al}_x\text{Ga}_{1-x}\text{As}$ ). In order to perform a correct comparison we derive a relationship between the 2D EG width (inversion layer width)  $a$  and the extension of the wave function in the bulk  $1/b$ . In the triangular-well approximation  $b$  is given by (see Ref. 8):

$$b^3 = \frac{48\pi e^2 m_z}{\epsilon_s \hbar^2} \left( N_d + \frac{11N_s}{32} \right), \quad (68)$$

where  $m_z$  is the effective mass perpendicular to the interface, which we assume everywhere equal to  $m^* = 0.067m_0$ ,  $\epsilon_s$  is the dielectric constant in the heterostructure,  $N_d$  is the 2D depletion layer concentration and  $N_s$  is the 2D electron concentration.

In order to derive this relationship we equalize the screening form factor as derived in Ref. 7 [see Eq. (8)] and the form factor given in Ref. 11 (see Appendix E).

We get the following relations corresponding to the first and the second case:

$$a = \frac{45}{8b} = \frac{16}{3b}. \quad (69)$$

Now we can compare correctly the results of our calculations using the value of the 2D EG width  $a$ , calculated by using the parameter set given in Ref. 11, Fig. 15. The spacer layer thickness  $s$  is assumed equal to the effective Bohr radius in our calculations. The semiclassical results for the 2D DOS obtained as a limiting case of the general path-integral expression for the DOS are plotted on the same graph with the results of multiple scattering theory in Fig. 19 against the energy in units of effective Rydbergs.

As can be seen from the figure, the semiclassical limit of the path-integral DOS is steeper than the multiple-scattering DOS and lies between their results for the same distance and at larger distances from the interface.

In Fig. 20 the low-energy band tail results for  $s = 2a_B^*$  corresponding to the second case are plotted together with

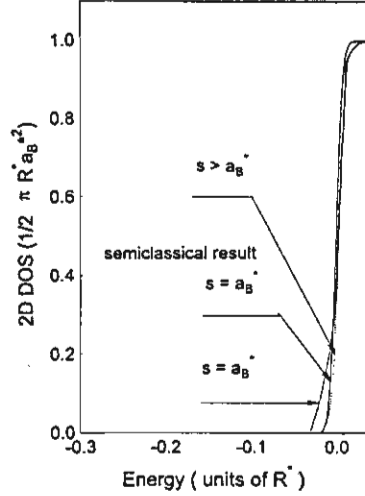


FIG. 19. Plot of the semiclassical normalized 2D DOS in units  $1/2\pi R a_B^{*2} = m^*/\pi\hbar^2$  vs energy in units of  $R^*$  (effective Rydberg) for  $s = a_B^*$  together with the results of multiple-scattering theory calculations for the same distance from the interface and for greater distances.

the semiclassical limit of the path-integration calculated DOS and the multiple-scattering theory results on a semi-logarithmic scale.

#### C. Tight-binding simulation of the white Gaussian noise problem, fluctuation theory results, and the white Gaussian noise limit of the path-integral 2D DOS

The DOS in the two-dimensional white Gaussian noise problem has been calculated from the coherent potential approximation at high energies, it has also been calculated from the fluctuation theory (method of Halperin and Lax<sup>16</sup>) in the low-energy band tail and it has been compared with

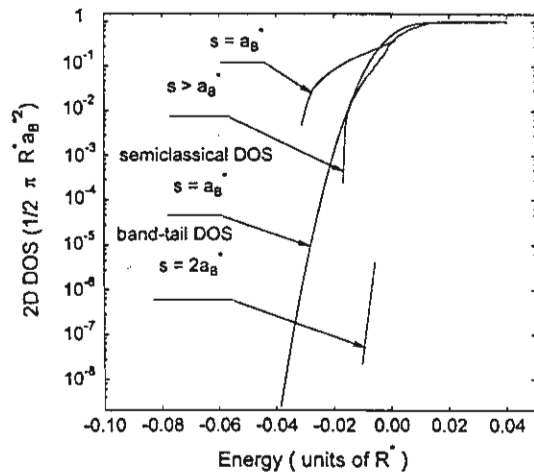


FIG. 20. Plot of the semiclassical normalized 2D DOS in units  $1/2\pi R a_B^{*2}$  vs energy in units of  $R^*$  (effective Rydberg) for  $s = a_B^*$  and band-tail DOS for  $s = 2a_B^*$  together with the results of multiple-scattering theory calculations for the same distance from the interface and for greater distances.

the results of a tight-binding 2D simulation with respect to the white noise problem.<sup>12</sup> In order to compare our results for the 2D DOS with the results of Ref. 12 it is necessary to take the strong screening limit of expression (40), which corresponds to the white Gaussian noise limit. We have already derived the expressions in the strong screening case (46), (A7) [and correspondingly for the second case, Eqs. (47), (A15)] for the dimensionless functions  $a(\nu)$  and  $b(\nu)$ . Normalizing the DOS with respect to the 2D free-electron DOS we get

$$\frac{\rho_1(\nu)}{\rho_0} = \frac{2\pi}{\xi_1^{3/2}} a(\nu) e^{-b(\nu)/2\xi_1} = \frac{2\pi}{\xi_2^{3/2}} a(\nu) e^{-b(\nu)/2\xi_2}, \quad (70)$$

where we have introduced once again the dimensionless parameters  $\xi_1$  and  $\xi_2$  as was done in (B1) and (B2).

The results for the normalized DOS of Ref. 12 have been presented as a function of the parameter

$$\eta = \frac{4\pi(E-E_0)}{Q}, \quad (71)$$

where  $Q$  is the energy scale of the white Gaussian noise problem given by

$$Q = \frac{2m^*}{\hbar^2} \int W(\mathbf{r}-\mathbf{r}') d^2\mathbf{r}'. \quad (72)$$

As has been pointed out in Ref. 12, for the tight-binding model this quantity is equivalent to

$$Q = \frac{w^2}{V}, \quad (73)$$

where  $w^2 = \xi_{q_s}' = \xi_{q_s}''$  is the dispersion of the random potential energy and  $V$  is the matrix element of the Hamiltonian that carries the electron from one site to its neighbor (assumed constant) in the tight-binding model with diagonalized disorder. The constant  $V$  represents the bandwidth and can be expressed in terms of the lattice constant  $a$ :

$$V = \frac{\hbar^2}{2m^*a^2}. \quad (74)$$

For the white Gaussian noise random potential the binary correlation function is given by

$$W(\mathbf{r}-\mathbf{r}') = \xi_L e^{-|\mathbf{r}-\mathbf{r}'|^2/L^2}, \quad (75)$$

where  $L$  is the correlation length of the random fluctuations.

The white Gaussian noise limit is equivalent to the strong screening case, therefore  $q_s = 1/L \rightarrow \infty$  (or equivalently  $L \rightarrow 0$ ). In performing this limiting procedure, since we consider a discrete lattice,  $L$  cannot be smaller than the lattice constant. Therefore we can take as a limiting value  $L = a$ ; i.e.,  $1/q_s = a$ . Substituting the last relation in Eq. (74) we get

$$V = \frac{\hbar^2 q_s^2}{2m^*} = E_{q_s}, \quad (76)$$

which means that the parameter  $V$  is equal to the kinetic energy associated with a region of the size of the inverse

screening length  $q_s$ . Thus, substituting Eq. (76) in Eq. (73) we obtain for the first and second case, respectively,

$$Q = \frac{\xi_{q_s}'}{E_{q_s}} = \frac{\xi_{q_s}''}{E_{q_s}}. \quad (77)$$

We can represent the argument  $\nu$  in Eq. (70) in terms of the parameter  $\eta$  from Eq. (71), thus obtaining

$$\nu = \frac{\eta \xi_1}{4\pi}. \quad (78)$$

Finally the following expression for the normalized DOS in the first case is obtained:

$$\frac{\rho_1(\eta)}{\rho_0} = \frac{1}{2\xi_1^{1/2}(sq_s)^2} \left( \frac{81.3^{5/2}}{2^{7/2}} \right) \eta \exp \left[ - \left( \frac{243}{128(sq_s)^2 \xi_1} + \frac{27\eta}{32\pi sq_s} \right) \right]. \quad (79)$$

Consider now the second case. Since the dimensionless energy is defined as  $\nu'' = (E_0 - E)/E_{q_s}$  [see Eq. (39)] from Eq. (71) we get that

$$\nu'' = \frac{\eta \xi_2}{4\pi}. \quad (80)$$

Comparing Eqs. (78) and (80) we obtain

$$\frac{\xi_1}{\xi_2} = \left( \frac{Q_s}{q_s} \right)^2. \quad (81)$$

Using Eq. (5) we obtain the following relationship between the two dimensionless parameters corresponding to the two cases.

$$\xi_1 = \xi_2 \left( \frac{2}{aq_s} \right). \quad (82)$$

The corresponding expression for the DOS in the strong screening limit is

$$\frac{\rho_1(\eta)}{\rho_0} = \frac{2\pi}{\xi_2^{3/2}} \left( a_1'' + a_2'' \xi_2 \frac{\eta}{4\pi} \right) \exp \left[ - \left( \frac{b_1''}{2\xi_2} + \frac{b_2'' \eta}{8\pi} \right) \right], \quad (83)$$

where the quantities  $a_1'', a_2'', b_1'', b_2''$  are functions of the dimensionless parameter  $sq_s$  and are given by Eq. (A15).

On the other hand we have to keep in mind that our results for the DOS as a function of the energy are obtained taking the average energy  $E_0$  as an unperturbed band edge while the results of Thouless *et al.*<sup>12</sup> have been plotted with respect to the CPA energy zero:

$$E_0 = -4V - \left( \frac{\xi}{4\pi V} \right) \left[ 1 + \ln \frac{128\pi V^2}{\xi} \right], \quad (84)$$

where we have introduced  $\xi$  as a general dispersion of the random potential energy. In the 2D case (because of the four nearest neighbors in the tight-binding model) the energy zero

of our path-integral DOS occurs (see Ref. 22 for the derivation in the one-dimensional case) at

$$E_0^* = -4V. \quad (85)$$

Introducing the dimensionless parameter  $\xi_1$  corresponding to the first case, we get for the energy zero shift

$$\Delta E = E_0^* - E_0 = \left( \frac{\xi_1 E_{q_2}}{4\pi} \right) \left[ 1 + \ln \left( \frac{128\pi}{\xi_1} \right) \right]. \quad (86)$$

The actual shift on the  $x$  axis is given by

$$4\pi \frac{\Delta E}{Q} = 1 + \ln \left( \frac{128\pi}{\xi_1} \right). \quad (87)$$

Taking into account the above considerations we have plotted the path-integral results for the 2D DOS in the white Gaussian limit of the second case on the same plot with the CPA high-energy DOS; the fluctuation band-tail DOS, obtained by using the Halperin and Lax method and the tight-binding simulations of the 2D DOS (Fig. 21).

As can be seen from Fig. 21 our path-integral results in the white Gaussian noise limit are very close to the tight-binding simulation points deep in the band tail. Moreover they are correctly shifted in contrast with the band-tail results from the fluctuation theory [see Ref. 12, Eq. (28)].

## VII. CONCLUSIONS

We have applied the path-integral method to the problem of 2D DOS calculation at the interface of a single  $\text{Al}_x\text{Ga}_{1-x}\text{As-GaAs}$  modulation-doped heterojunction. Analytical expressions for the 2D band-tail DOS in the two limiting cases of a weak and a strong screening as well as in the semiclassical limit have been derived, thus obtaining asymptotic expressions for the whole energy range. These results have been compared to other theoretical approaches of the DOS calculation in two dimensions. It has been found that the semiclassical Kane limit of the path-integral DOS leads exactly to the expression obtained by using the generalized semiclassical approach<sup>10</sup> as well as leading to very similar results obtained by using the multiple-scattering theory.<sup>11</sup> On the other hand, the white Gaussian noise limit of our band-tail DOS expression has been found to fit quite well to the data from the tight-binding simulations.<sup>12</sup> This confirms the ability of the path-integration method to correctly obtain the DOS in the whole energy range in two dimensions.

Numerical results have been presented for a single  $\text{Al}_x\text{Ga}_{1-x}\text{As-GaAs}$  modulation-doped heterojunction and the effects of varying its relevant parameters have been thoroughly studied in two limiting cases of the general correlation function thereby accounting for the statistical properties of the impurity charge distribution. It should be noted that the expressions of the 2D DOS obtained are general and could be applied to any heterojunction with hydrogenic impurity type and parabolic conduction (valence) subband.

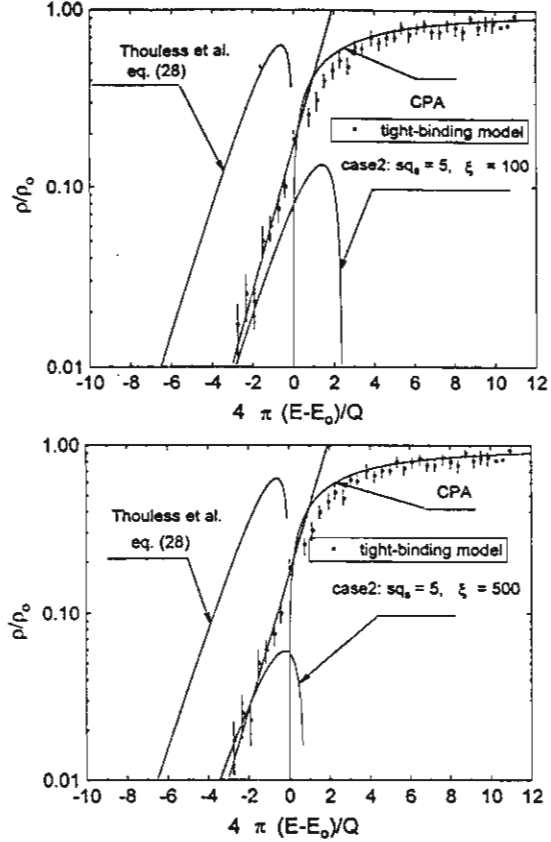


FIG. 21. Plot of the white Gaussian limit in the second case of the path-integral expression for the 2D DOS as a function of the normalized parameter  $\eta = 4\pi(E - E_0)/Q$  for two different values of the dispersion  $\xi_2 = 100, 500$  at a fixed value of the dimensionless parameter  $sQ_2 = 5$ . The straight line represents a fit to the tight-binding simulation results [Ref. 12, Eq. (31)]. The analytical expression for the high-energy DOS from the CPA method and the band-tail DOS inferred from fluctuation theory [Ref. 12, Eq. (28)] are plotted as well.

## ACKNOWLEDGMENTS

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## APPENDIX A

Let us consider the first case, corresponding to  $s q_2 \gg 1$  and  $a q_2 \ll 1$ . For a weak screening  $\nu \gg 1$  ( $q_2 \rightarrow 0$  or equivalently  $z \rightarrow 0$ ) Eq. (43) can be simplified to the following cubic equation:

$$4\nu z^3 - 2\nu(1 + 2s q_2)z^2 + 6s q_2 = 0, \quad (A1)$$

whose real root can be expanded around the infinity energy point ( $\nu \gg 1$ ) leading to

$$z \approx \frac{1}{2} (1 + 2sq_s) - \frac{6sq_s[1 - 6sq_s - 12(sq_s)^2 - 8(sq_s)^3]}{(1 + 2sq_s)^5} \frac{1}{\nu}. \quad (\text{A2})$$

Substituting this solution in Eqs. (41) and (42), expanding around infinity, and taking into account the inequality  $sq_s \gg 1$ , we obtain the following expressions in the weak screening case:

$$a(\nu) \approx \frac{9\nu}{2^{3/2}(sq_s)^2}, \quad (\text{A3})$$

$$b(\nu) \approx \pi\nu^2.$$

In the strong screening case since  $\nu \ll 1$  ( $q_s \rightarrow \infty$  or equivalently  $z \rightarrow \infty$ ) we can simplify the expression for  $b(\nu, z) \approx (3/4z + \nu)^2 / 1 - 1/2sq_s + z/sq_s$ , which, after taking the derivative, leads to a quadratic equation

$$4\nu z^2 + 9z + 6sq_s - 3 = 0. \quad (\text{A4})$$

Expanding the positive root of the above equation around the  $\nu=0$  point we obtain the following approximate solution for  $z$ :

$$z \approx \frac{1}{3} (1 - 2sq_s) - \frac{(1 - 2sq_s)^2}{324} \nu \quad (\text{A5})$$

from which, after substituting in Eqs. (41) and (42) and expanding around the zero energy point, we obtain the following expressions in the strong screening limit:

$$a(\nu) \approx a'_1 + a'_2 \nu, \quad (\text{A6})$$

$$b(\nu) \approx b'_1 + b'_2 \nu,$$

where the following notations have been introduced:

$$a'_1 = \frac{729\nu^{3/2}}{128(sq_s)^3}, \quad b'_1 = \frac{243}{64(sq_s)^2}, \quad (\text{A7})$$

$$a'_2 = \frac{81.3^{5/2}}{2^{1/2}(sq_s)^2}, \quad b'_2 = \frac{27}{4sq_s}.$$

Analogously, for the second case, namely,  $sq_s \gg 1$  and  $aq_s \gg 1$  in the weak screening limit, after setting  $\nu \gg 1$  ( $Q_s \rightarrow 0$  or equivalently  $z \rightarrow 0$ ), we get the following cubic equation:

$$2\nu z^3 + 2(sq_s)^2[(1 - 2w)\nu + 2sq_s u]z^2 + 3(sq_s)^2(2sq_s u - 1) = 0, \quad (\text{A8})$$

which can be simplified (taking into account that  $sq_s \gg 1$  and therefore  $u \approx 0$ ,  $w \approx 0$ ) to

$$2\nu z^3 + 2(sq_s)^2\nu z^2 - 3(sq_s)^2 = 0, \quad (\text{A9})$$

whose real root after expanding around the infinite energy point becomes

$$z \approx -(sq_s)^2 + \frac{3}{2(sq_s)^2} \frac{1}{\nu}. \quad (\text{A10})$$

After substitution in the simplified expression for  $a(\nu, z)$  and  $b(\nu, z)$  in the limit as  $z \rightarrow 0$ , we get the following expressions in the weak screening limit:

$$a(\nu) \approx \frac{9}{2^3(sq_s)^4}, \quad (\text{A11})$$

$$b(\nu) \approx 2\pi\nu^2.$$

In the strong screening case  $\nu \ll 1$  ( $Q_s \rightarrow \infty$  or equivalently  $z \rightarrow \infty$ ) Eq. (44) can be simplified to the following quadratic equation:

$$4\nu z^2 + 3z - 6 = 0, \quad (\text{A12})$$

whose positive root is

$$z \approx 2 - \frac{16}{3}\nu. \quad (\text{A13})$$

After substituting the above root in the expressions (41) and (42) and expanding around the point  $\nu=0$  we get the following expressions in the strong screening limit of the second case

$$a(\nu) \approx a''_1 + a''_2 \nu, \quad (\text{A14})$$

$$b(\nu) \approx b''_1 + b''_2 \nu,$$

where the following constants have been introduced:

$$a''_1 = \frac{27}{256[e^2(1 - 2sq_s u) - 4w]},$$

$$b''_1 = \frac{9}{64[e^2(1 - 2sq_s u) - 4w]}, \quad (\text{A15})$$

$$a''_2 = \frac{27}{16} \frac{e^2(1 - 2sq_s u) - 10w}{[e^2(1 - 2sq_s u) - 4w]^2},$$

$$b''_2 = \frac{9e^2(1 - 2sq_s u) - 30w}{4[e^2(1 - 2sq_s u) - 4w]^2}.$$

## APPENDIX B

Similar to Ref. 23 we introduce a reduced parameter for the first and the second case, respectively,

$$\xi_1 = \frac{\xi'_{q_s}}{E_{q_s}^2} = \frac{\xi'}{sq_s E_{q_s}^2}, \quad (\text{B1})$$

where  $\xi'$  is given by Eq. (31) and  $\xi'_{q_s} = \xi'/sq_s$  in the first case

$$\xi_2 = \frac{\xi''_{Q_s}}{E_{Q_s}^2}, \quad (\text{B2})$$

where  $\xi''_{Q_s}$  is given by Eq. (32).

The so introduced parameters represent a measure for the magnitude of the fluctuations of the random potential.

Let us express the band-tail DOS in the first case in units of  $[Q_s^2/E_Q, \xi_2^{3/2}]$ . Using the relation between the 2D EG and 3D inverse screening lengths given by Eq. (5) we obtain

$$\frac{\rho_1^{(1)}(\nu)}{Q_s^2/E_Q, \xi_2^{3/2}} = \left(\frac{\xi_2}{\xi_1}\right)^{3/2} a(\nu, z) \exp\left(-\frac{b(\nu, z)}{2\xi_1}\right) \quad (\text{B3})$$

and correspondingly

$$\frac{\rho_1^{(2)}(\nu)}{Q_s^2/E_Q, \xi_2^{3/2}} = a(\nu, z) \exp\left(-\frac{b(\nu, z)}{2\xi_2}\right). \quad (\text{B4})$$

After substituting  $\xi_1$  and  $\xi_2$  from (B1) and (B2) and using the definitions for the random potential energy dispersions from Eqs. (31) and (32) we obtain

$$\frac{\xi_2}{\xi_1} = \frac{saq_s^2}{16}, \quad (\text{B5})$$

which substituted in Eq. (B3) gives

$$\frac{\rho_1^{(1)}(\nu)}{Q_s^2/E_Q, \xi_2^{3/2}} = \left(\frac{saq_s^2}{16}\right)^{3/2} a(\nu, z) \exp\left(-\frac{b(\nu, z)saq_s^2}{16\xi_2}\right). \quad (\text{B6})$$

#### APPENDIX C

Consider first the band-tail expression for the DOS given by Eq. (40). Let us define the dimensionless parameters  $\xi_1$  and  $\xi_2$  according to Eqs. (B1) and (B2). The DOS in the band tail can be rewritten as

$$\rho_1^{\text{BT}}(\nu) = \begin{cases} \frac{q_s^2}{E_{q_s} \xi_1^{3/2}} a(\nu, z) e^{-b(\nu, z)/2\xi_1} \\ \frac{Q_s^2}{E_{Q_s} \xi_2^{3/2}} a(\nu, z) e^{-b(\nu, z)/2\xi_2} \end{cases} \quad (\text{C1})$$

Let us consider now the semiclassical expressions (56) and similarly introduce dimensionless energy according to Eq. (39) and the parameters:

$$\xi_{q_s}'' = \frac{\xi_{q_s}}{E_{q_s}^2} \quad (\text{C2})$$

and

$$\xi_{Q_s}''' = \frac{\xi_{Q_s}}{E_{Q_s}^2}. \quad (\text{C3})$$

Consider the first case. Using Eqs. (B1), (54), and (C2) we get that

$$\rho_1^{sc}(\nu) = \frac{2m^*}{(2\pi)^{3/2} \hbar^2} e^{-\nu^2 \pi / \xi_1} D_{-1}\left(\frac{\nu \sqrt{4\pi}}{\sqrt{\xi_1}}\right). \quad (\text{C4})$$

From Eq. (C1) the band-tail DOS in units of  $q_s^2/E_{q_s} \xi_1^{3/2}$  is given by

$$\rho_1^{\text{BT}}(\nu) = a(\nu, z) e^{-b(\nu, z)/2\xi_1}. \quad (\text{C5})$$

Representing the semiclassical DOS in the same units we get that

$$\rho_1^{sc}(\nu) = \left(\frac{\xi_1}{2\pi}\right)^{3/2} e^{-\nu^2 \pi / \xi_1} D_{-1}\left(\frac{2\nu \sqrt{\pi}}{\sqrt{\xi_1}}\right). \quad (\text{C6})$$

Using the second equality of (B1) we finally get both expressions for the DOS as a function of the dimensionless energy  $\nu$  depending on the same parameter set, namely,  $sq_s, \xi_1$ , in order to be compared

$$\rho_1^{sc}(\nu) = \left(\frac{\xi_1 sq_s}{2\pi}\right)^{3/2} e^{-\nu^2 \pi / \xi_1 sq_s} D_{-1}\left(\frac{2\nu \sqrt{\pi}}{\sqrt{\xi_1 sq_s}}\right). \quad (\text{C7})$$

$$\rho_1^{\text{BT}}(\nu) = a(\nu, z) e^{-b(\nu, z)sq_s/2\xi_1}. \quad (\text{C8})$$

Let us consider now the second case. Analogously, from Eqs. (B2), (55), and (C3) we get

$$\rho_1^{sc}(\nu) = \frac{2m^*}{(2\pi)^{3/2} \hbar^2} e^{-\nu^2 \pi / 2\xi_2(1-2suQ_s)} \times D_{-1}\left(\frac{\nu \sqrt{2\pi}}{\sqrt{\xi_2(1-2suQ_s)}}\right). \quad (\text{C9})$$

On the other hand, the band-tail DOS in the second case in units of  $Q_s^2/E_{Q_s} \xi_2^{3/2}$  is given by

$$\rho_1^{\text{BT}}(\nu) = a(\nu, z) e^{-b(\nu, z)/2\xi_2}. \quad (\text{C10})$$

Representing the semiclassical expression for the DOS in the same units we get

$$\rho_1^{sc}(\nu) = \left(\frac{\xi_2}{2\pi}\right)^{3/2} e^{-\nu^2 \pi / 2\xi_2(1-2suQ_s)} \times D_{-1}\left(\frac{\nu \sqrt{2\pi}}{\sqrt{\xi_2(1-2suQ_s)}}\right). \quad (\text{C11})$$

#### APPENDIX D

Let us define the 2D impurity density as

$$n_2 = n_1 d \quad (\text{D1})$$

and the dimensionless density  $\nu^*$  and the dimensionless energy  $E^*$  according to Ref. 10:

$$\nu^* = \frac{2\pi n_2}{k_{2n}^2}, \quad (\text{D2})$$

$$E^* = \frac{2\pi \epsilon_2}{e^2} E. \quad (\text{D3})$$

We can identify the zero-temperature inverse screening length of a noninteracting Fermi gas  $k_{2n}$  with the 2D inverse

screening length  $q_s = 2/a_g^*$  introduced by Ando *et al.*<sup>8</sup> On the other hand, we have introduced the dimensionless energy  $\nu$  for our problem according to Eq. (39). Substituting in Eq. (D3) the energy  $E$  from Eq. (39) and the expression for  $E_{q_s}$ , we obtain  $E^* = \nu$ , which means that we can identify the dimensionless energy with the one previously defined and rewrite the first case DOS expression (40) as<sup>24</sup>

$$\rho_1(E^*) = \frac{(E_{q_s} q_s)^2}{\xi_{q_s}^{1/2}} a(E^*, z) e^{-b(E^*, z)(E_{q_s}^2/2\xi_{q_s})}. \quad (D4)$$

Let us define a dimensionless parameter, according to

$$\eta = \frac{E^*}{\sqrt{\nu^*}}. \quad (D5)$$

Its normalization with respect to the free-electron density in 2D can be represented in terms of the newly introduced parameter by

$$\left(\frac{\pi \hbar^2}{m^*}\right) \rho_1(\eta) = \frac{2\pi}{4^{3/2}(q_s a^2/2\pi s)^{3/2}} \eta^3 a(\eta, z) \times e^{-b(\eta, z) \eta^2 16\pi s/q_s a^2}. \quad (D6)$$

It is convenient to introduce a new dimensionless parameter by

$$\eta^* = \eta \left( \frac{\pi s}{q_s a^2} \right)^{1/2}. \quad (D7)$$

And finally we get in the band tail:

$$\left(\frac{\pi \hbar^2}{m^*}\right) \rho_1(\eta^*) = \left(\frac{2^{5/2}\pi}{4^3}\right) \eta^{*3} a(\eta^*, z) e^{-b(\eta^*, z) 16\eta^{*2}}. \quad (D8)$$

The normalized 2D semiclassical expression is correspondingly

$$\left(\frac{\pi \hbar^2}{m^*}\right) \rho_{2n}(\eta^*) = \frac{1}{2} [1 + \text{erf}(\eta^*)]. \quad (D9)$$

## APPENDIX E

The form factor of Ref. 11 is given by

$$F_C(q) = \frac{1 + 9q/8b + 3q^2/8b^2}{(1 + q/b)^3}. \quad (E1)$$

In the first case ( $sq_s \gg 1$ ,  $aq_s \ll 1$ ) we can expand Eq. (8) up to the third-order term leading to

$$F(q) \approx 1 - \frac{1}{3} a q. \quad (E2)$$

Expanding (E1) as well and taking into account that  $aq_s \ll 1$ , which is equivalent to  $q/b \ll 1$ , we get that

$$F_C(q) \approx 1 - \frac{15}{8} \frac{q}{b}. \quad (E3)$$

Equalizing the coefficients before the equal powers of the two polynomials, we obtain

$$a = \frac{45}{8b}. \quad (E4)$$

Analogously, in the opposite case  $aq_s \gg 1$ , which is equivalent to  $q/b \gg 1$ , we get that

$$a = \frac{16}{3b}. \quad (E5)$$

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Wilrijk, July 8 1998

Prof. A. KANANTHAI  
Department of Mathematics  
Chiangmai University

Chiangmai 50200  
THAILAND

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# On the Convolution Equation Related to the Diamond Kernel of Marcel Riesz

AMNUAY KANANTHAI

**ABSTRACT.** In this paper, we study the distribution  $e^{\alpha t} \diamond^k \delta$  where  $\diamond^k$  is introduced and named as the Diamond operator iterated k-times ( $k = 0, 1, 2, \dots$ ) and is defined by

$$\diamond^k = \left( \left( \frac{\partial^2}{\partial t_1^2} + \frac{\partial^2}{\partial t_2^2} + \dots + \frac{\partial^2}{\partial t_p^2} \right)^2 - \left( \frac{\partial^2}{\partial t_{p+1}^2} + \frac{\partial^2}{\partial t_{p+2}^2} + \dots + \frac{\partial^2}{\partial t_{p+q}^2} \right)^2 \right)^k$$

where  $t = (t_1, t_2, \dots, t_n)$  is a variable and  $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_n)$  is a constant and both are the points in the  $n$  - dimensional Euclidean space  $R^n$ ,  $\delta$  is the Dirac-delta distribution with  $\diamond^0 \delta = \delta$  and  $p + q = n$  (the dimension of  $R^n$ )

At first, the properties of  $e^{\alpha t} \diamond^k \delta$  are studied and later we study the application of  $e^{\alpha t} \diamond^k \delta$  for solving the solutions of the convolution equation

$$(e^{\alpha t} \diamond^k \delta) * u(t) = e^{\alpha t} \sum_{r=0}^m c_r \diamond^r \delta$$

We found that its solutions related to the Diamond Kernel of Marcel Riesz and moreover, the type of solutions such as, the classical solution (the ordinary function) or the tempered distributions depending on  $m, k$  and  $\alpha$ .

Keywords : Diamond operator, Kernel of Marcel Riesz, Dirac delta distributions, Tempered distribution

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## 1. INTRODUCTION

From A. Kananthai [2, Theorem 3.1 ], the equation  $\diamond^k u(t) = \delta$  has  $(-1)^k S_{2k}(t) * R_{2k}(t)$  as an elementary solution and is called the Diamond Kernel of Marcel Riesz where  $S_{2k}(t)$  and  $R_{2k}(t)$  are defined by (2.1) and (2.2) respectively with  $\gamma = 2k$  where  $\gamma$  is nonnegative.

Consider the convolution equation

$$(e^{\alpha t} \diamond^k \delta) * u(t) = e^{\alpha t} \sum_{r=0}^m c_r \diamond^r \delta \quad (1.1)$$

In finding the type of solutions  $u(t)$  of (1.1), we use the method of convolution of the tempered distribution. Before going to that point, some definitions and basic concepts are needed.

## 2. Preliminaries

**Definition 2.1** Let the function  $S_\gamma(t)$  be defined by

$$S_\gamma = 2^{-\gamma} \pi^{-n/2} \Gamma\left(\frac{n-\gamma}{2}\right) \frac{|t|^{\gamma-n}}{\Gamma(\frac{\gamma}{2})} \quad (2.1)$$

where  $\gamma$  is a complex parameter,  $n$  is the dimension of  $R^n$ ,  $t = (t_1, t_2, \dots, t_n) \in R^n$  and  $|t| = \sqrt{(t_1^2 + \dots + t_n^2)}$ . Now  $S_\gamma$  is an ordinary function if  $Re(\gamma) \geq n$  and is a distribution of  $\gamma$  if  $Re(\gamma) < n$ .

**Definition 2.2** Let  $t = (t_1, t_2, \dots, t_n)$  be the point of  $R^n$  and write  $v = t_1^2 + t_2^2 + \dots + t_p^2 - t_{p+1}^2 - t_{p+2}^2 - \dots - t_{p+q}^2$ ,  $p+q = n$ . Denote by  $\Gamma_+ = \{t \in R^n : t_1 > 0 \text{ and } v > 0\}$  the set of an interior of the forward cone and  $\bar{\Gamma}$  is the closure of  $\Gamma$ .

For any complex number  $\gamma$ , define

$$R_\gamma(t) = \begin{cases} \frac{V^{(\gamma-n)/2}}{K_n(\gamma)}, & \text{if } t \in \Gamma_+ \\ 0, & \text{if } t \notin \Gamma_+ \end{cases}$$

where  $K_n(\gamma)$  is given by the formula

$$K_n(\gamma) = \frac{\pi^{(n-1)/2} \Gamma(\frac{2+\gamma-n}{2}) \Gamma(\frac{1-\gamma}{2}) \Gamma(\gamma)}{\Gamma(\frac{2+\gamma-p}{2}) \Gamma(\frac{p-\gamma}{2})}$$

The function  $R_\gamma(t)$  was introduced by Nozaki [3, p.72]. It is well known that  $R_\gamma(t)$  is an ordinary function if  $\operatorname{Re}(\gamma) \geq n$  and is a distribution of  $\alpha$  if  $\operatorname{Re}(\gamma) < n$ . Let  $\operatorname{supp} R_\gamma(t)$  denote the support of  $R_\gamma(t)$  and suppose that  $\operatorname{supp} R_\gamma(t) \subset \bar{\Gamma}_+$ .

**Lemma 2.1**  $S_\gamma(t)$  and  $R_\gamma(t)$  are homogeneous distributions of order  $\alpha - n$ . Moreover they are tempered distribution.

**Proof.** Since  $S_\gamma(t)$  and  $R_\gamma(t)$  satisfy the Euler equation

$$\sum_{i=1}^n t_i \frac{\partial R_\gamma(t)}{\partial t_i} = (\alpha - n) R_\gamma(t)$$

$$\sum_{i=1}^n t_i \frac{\partial S_\gamma(t)}{\partial t_i} = (\alpha - n) S_\gamma(t)$$

then they are homogeneous distribution of order  $\alpha - n$  by W.F. Donoghue [1, p 154 -155] that proved that every homogeneous distribution is a tempered distribution.  $\square$

**Lemma 2.2** (The convolution of tempered distribution) The convolution  $S_\gamma(t) * R_\gamma(t)$  exists and is a tempered distribution.

**Proof.** Choose  $\operatorname{supp} R_\gamma(t) = K \subset \bar{\Gamma}_+$  where  $K$  is a compact set. Then  $R_\gamma(t)$  is a tempered distribution with compact support and by W.F Donoghue [1, p 156 - 159],  $S_\gamma(t) * R_\gamma(t)$  exists and is a tempered distribution.  $\square$

### 3. The properties of $e^{\alpha t} \diamond^k \delta$

**Lemma 3.1**

$$e^{\alpha t} \Diamond^k \delta = L^k \delta \quad (3.1)$$

where  $L$  is the partial differential operator of Diamond type and is defined by

$$\begin{aligned} L \equiv & \Diamond + \sum_{r=1}^n \alpha_r^2 \square - 2 \sum_{r=1}^n \sum_{i=1}^r (\alpha_r \frac{\partial^3}{\partial t_i^2 \partial t_r} + \alpha_i \frac{\partial^3}{\partial t_i \partial t_r^2}) \\ & + 2 \sum_{r=1}^n \sum_{j=p+1}^{p+q} (\alpha_r \frac{\partial^3}{\partial t_j^2 \partial t_r} + \alpha_j \frac{\partial^3}{\partial t_j \partial t_r^2}) \\ & + 4 (\sum_{r=1}^n \sum_{i=1}^p \alpha_r \alpha_j \frac{\partial^2}{\partial t_i \partial t_r} - \sum_{r=1}^n \sum_{j=p+1}^{p+q} \alpha_r \alpha_j \frac{\partial^2}{\partial t_j \partial t_r}) \\ & - 2 \sum_{r=1}^n \alpha_r^2 (\sum_{i=1}^p \alpha_i \frac{\partial}{\partial t_i} - \sum_{j=p+1}^{p+q} \alpha_j \frac{\partial}{\partial t_j}) \\ & + (\sum_{i=1}^p \alpha_i^2 - \sum_{j=p+1}^{p+q} \alpha_j^2) \Delta - 2 (\sum_{i=1}^p \alpha_i^2 - \sum_{j=p+1}^{p+q} \alpha_j^2) \sum_{r=1}^n \alpha_r \frac{\partial}{\partial t_r} \\ & + (\sum_{i=1}^p \alpha_i^2 - \sum_{j=p+1}^{p+q} \alpha_j^2) \sum_{r=1}^n \alpha_r^2 \end{aligned} \quad (3.2)$$

where  $\square = \sum_{i=1}^p \frac{\partial^2}{\partial t_i^2} - \sum_{j=p+1}^{p+q} \frac{\partial^2}{\partial t_j^2}$ ,  $\Delta = \sum_{i=1}^p \frac{\partial^2}{\partial t_i^2}$ ,  $p+q=n$ . Actually  $\Diamond = \square \Delta$  and  $e^{\alpha t} \Diamond^k \delta$  is a tempered distribution of order  $4k$ .

**Proof.** For  $k=1$ , we have

$$\langle e^{\alpha t} \Diamond \delta, \varphi(t) \rangle = \langle \delta, \Diamond e^{\alpha t} \varphi(t) \rangle$$

where  $\varphi(t) \in \mathcal{S}$  the Schwartz space. By computing directly we obtain

$$\Diamond e^{\alpha t} \varphi(t) = e^{\alpha t} M \varphi(t) \quad (3.3)$$

where  $M$  is the partial differential operator of the form (3.2) whose the coefficients of the 3<sup>rd</sup> term, the 4<sup>th</sup> term, the 6<sup>th</sup> term and the 8<sup>th</sup> term of the right hand side of (3.2) have opposite signs.

Thus  $\langle \delta, \Diamond e^{\alpha t} \varphi(t) \rangle = \langle \delta, e^{\alpha t} M \varphi(t) \rangle = M \varphi(0)$ .

By the properties of  $\delta$  and its partial derivatives with the linear differential operator  $M$ , we obtain  $M\varphi(0) = \langle L\delta, \varphi \rangle$  where  $L$  defined by (3.2). It follows that  $e^{\alpha t} \diamond \delta = L\delta$ . Now

$$\underbrace{(e^{\alpha t} \diamond \delta) * (e^{\alpha t} \diamond \delta) * \dots * (e^{\alpha t} \diamond \delta)}_{k\text{-times}} = \underbrace{(L\delta) * (L\delta) * \dots * (L\delta)}_{k\text{-times}}$$

we have  $e^{\alpha t}(\delta * \diamond^k \delta) = \delta * (L^k \delta)$ . Thus  $e^{\alpha t} \diamond^k \delta = L^k \delta$ . It follows that, for any  $k$ , we obtain (3.1). Since  $\delta$  has a compact support, hence by L. Schwartz [4],  $\delta$  and  $L^k \delta$  are tempered distributions and  $L^k \delta$  has order  $4k$ . It follows that  $e^{\alpha t} \diamond^k \delta$  is a tempered distribution of order  $4k$ .  $\square$

**Lemma 3.2** (*Boundedness property*)

$|\langle e^{\alpha t} \diamond^k \delta, \varphi(t) \rangle| \leq K$  where  $K$  is a constant and  $\varphi \in S$ .

**Proof.**

$$\begin{aligned} \langle e^{\alpha t} \diamond^k \delta, \varphi(t) \rangle &= \langle \diamond^k \delta, e^{\alpha t} \varphi(t) \rangle \\ &= \langle \diamond^{k-1} \delta, \diamond e^{\alpha t} \varphi(t) \rangle \\ &= \langle \diamond^{k-1} \delta, e^{\alpha t} M \varphi(t) \rangle \end{aligned}$$

where  $M$  is defined by (3.3). By keeping on operate  $\diamond$   $k - 1$  times we obtain

$$\begin{aligned} \langle e^{\alpha t} \diamond^k \delta, \varphi(t) \rangle &= \langle \delta, e^{\alpha t} M^k \varphi(t) \rangle \\ &= M^k \varphi(0). \end{aligned}$$

Since  $\varphi(0)$  is bounded and also  $M^k \varphi(0)$  is bounded. It follows that  $|\langle e^{\alpha t} \diamond^k \delta, \varphi(t) \rangle| = |M^k \varphi(0)| \leq K$ .  $\square$

#### 4. The Application of $e^{\alpha t} \diamond^k \delta$

Given  $u(t)$  is an distribution and by Lemma 3.1, we have

$$(e^{\alpha t} \diamond^k \delta) * u(t) = (L^k \delta) * u(t) = L^k u(t)$$

where  $L$  is defined by (3.2).

**Theorem 4.1** *Given the linear partial differential equation of the form*

$$(e^{\alpha t} \diamond^k \delta) * u(t) = L^k u(t) = \delta \quad (4.1)$$

*Then  $u(t) = e^{\alpha t} (-1)^k S_{2k}(t) * R_{2k}(t)$  is an elementary solution of (4.1) or The Diamond Kernel of Marcel Riesz of (4.1) where  $S_{2k}(t)$  and  $R_{2k}(t)$  are defined by (2.1) and (2.2) respectively with  $\gamma = 2k$ .*

**Proof.** By A. Kananthai [2, Lemma 2.4],  $(-1)^k S_{2k}(t)$  is an elementary solution of the Laplace operator  $\Delta^k$  iterated  $k$ -times and also by S.E. Trione [5],  $R_{2k}(t)$  is an elementary solution of the ultra-hyperbolic operator  $\square^k$  iterated  $k$ -times (that is  $\Delta^k (-1)^k S_{2k}(t) = \delta$  and  $\square^k R_{2k}(t) = \delta$ ).

Now  $\diamond^k = \square^k \Delta^k$ , consider  $e^{\alpha t} (\square^k \Delta^k \delta) * R_{2k}(t) = \delta$  By Lemma 2.2 with  $\gamma = 2k$ ,  $(-1)^k S_{2k}(t) * R_{2k}(t)$  exists and is a tempered distribution.

Convolving both sides of the above equation by  $e^{\alpha t} [(-1)^k S_{2k}(t) * R_{2k}(t)]$  we obtain

$$e^{\alpha t} [\Delta^k (-1)^k S_{2k}(t) * \square^k R_{2k}(t) * u(t)] = [e^{\alpha t} (-1)^k S_{2k}(t) * R_{2k}(t)] * \delta$$

$$(e^{\alpha t} \delta) * u(t) = e^{\alpha t} (-1)^k S_{2k}(t) * R_{2k}(t)$$

It follows that  $u(t) = e^{\alpha t} (-1)^k S_{2k}(t) * R_{2k}(t)$ . □

**Theorem 4.2** *Given the convolution equation*

$$(e^{\alpha t} \diamond^k \delta) * u(t) = e^{\alpha t} \sum_{r=0}^m c_r \diamond^r \delta \quad (4.2)$$

*then the type of solutions of (4.2) depend on the relationship between  $k$ ,  $m$  and  $\alpha$  are as the following cases.*

- (1) *If  $m < k$  and  $m = 0$  then (4.2) has the solution  $u(t) = e^{\alpha t} [c_0 (-1)^k S_{2k}(t) * R_{2k}(t)]$  and  $u(t)$  is an ordinary function for  $2k \geq n$  with any  $\alpha$  and is a tempered distribution for  $2k < n$  and for some  $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_n)$  with  $\alpha_i < 0 (i = 1, 2, \dots, n)$ .*
- (2) *If  $0 < m < k$ , then the solution of (4.2) is*

$$u(t) = e^{\alpha t} \left[ \sum_{r=1}^m c_r (-1)^{k-r} S_{2k-2r}(t) * R_{2k-2r}(t) \right]$$

which is an ordinary function for  $2k - 2r \geq n$  with any  $\alpha$  and is a tempered distribution if  $2k - 2r < n$  for some  $\alpha$  with  $\alpha_i < 0 (i = 1, 2, \dots, n)$ .

(3) If  $m \geq k$  and for any  $\alpha$  and suppose that  $k \leq m \leq M$ , then (4.2) has  $u(t) = e^{\alpha t} \sum_{r=k}^M c_r \diamond^{r-k} \delta$  as a solution which is the singular distribution.

Proof. (1) For  $m < k$  and  $m = 0$ , then (4.2) becomes  $(e^{\alpha t} \diamond^k \delta) * u(t) = e^{\alpha t} C_0 \delta = C_0 e^{\alpha t} \delta = C_0 \delta$ . By Theorem 4.1 we obtain

$$u(t) = C_0 e^{\alpha t} ((-1)^k S_{2k}(t) * R_{2k}(t))$$

Now, by (2.1) and (2.2)  $S_{2k}(t)$  and  $R_{2k}(t)$  are ordinary functions respectively for  $2k \geq n$ . It follows that  $u(t)$  is an ordinary function for any constant  $\alpha$ . If  $2k < n$  then  $S_{2k}(t)$  and  $R_{2k}(t)$  are the analytic functions except at the origin and by Lemma 2.1  $S_{2k}(t)$  and  $R_{2k}(t)$  are tempered distributions and by Lemma 2.2,  $(-1)^k S_{2k}(t) * R_{2k}(t)$  exists and is a tempered distribution.

Now, for some  $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_n)$  with  $\alpha_i < 0 (i = 1, 2, \dots, n)$  we have  $e^{\alpha t}$  is a slow growth function and also its partial derivative is a slow growth. It follows that  $e^{\alpha t} [(-1)^k S_{2k}(t) * R_{2k}(t)]$  is also a tempered distribution.

(2) for  $0 < m < k$ , we have

$$(e^{\alpha t} \diamond^k \delta) * u(t) = e^{\alpha t} [c_1 \diamond \delta + c_2 \diamond^2 \delta + \dots + c_m \diamond^m \delta].$$

Convolving both sides by  $e^{\alpha t} [(-1)^k S_{2k}(t) * R_{2k}(t)]$ , we obtain

$$\begin{aligned} u(t) &= e^{\alpha t} [c_1 \diamond ((-1)^k S_{2k}(t) * R_{2k}(t)) + c_2 \diamond^2 ((-1)^k S_{2k}(t) * R_{2k}(t)) \\ &\quad + \dots + c_m \diamond^k ((-1)^k S_{2k}(t) * R_{2k}(t))] \\ &= e^{\alpha t} [c_1 (-1)^{k-1} S_{2k-2}(t) * R_{2k-2}(t) + c_2 (-1)^{k-2} S_{2k-4}(t) * R_{2k-4}(t) \\ &\quad + \dots + c_m (-1)^{k-m} S_{2k-2m}(t) * R_{2k-2m}(t)] \\ &= e^{\alpha t} \left[ \sum_{r=1}^m (-1)^{k-r} S_{2k-2r}(t) * R_{2k-2r}(t) \right] \end{aligned}$$

by Theorem 4.1 and by A. Kananthai [2, Theorem 3.2] for  $r < k$ . Similarly, as in the case (1)  $e^{\alpha t} \left[ \sum_{r=1}^m (-1)^{k-r} S_{2k-2r}(t) * R_{2k-2r}(t) \right]$  is the ordinary function if  $2k - 2r \geq n$

and for any  $\alpha$ , and is a tempered distribution if  $2k - 2r < n$  and for some  $\alpha$  with  $\alpha_i < 0 (i = 1, 2, \dots, n)$ .

(3) For  $m \geq k$  and for any  $\alpha$ , suppose that  $k \leq m \leq M$  we have

$$(e^{\alpha t} \diamond^k \delta) * u(t) = c_k e^{\alpha t} \diamond^k \delta + c_{k+1} e^{\alpha t} \diamond^{k+1} \delta + \dots + c_M e^{\alpha t} \diamond^M \delta.$$

Convolving both sides by  $e^{\alpha t}((-1)^k S_{2k}(t) * R_{2k}(t))$  and by A. Kananthai [2, Theorem 3.2] for  $k \leq m \leq M$ , we obtain

$$u(t) = c_k e^{\alpha t} \delta + c_{k+1} e^{\alpha t} \diamond \delta + c_{k+2} e^{\alpha t} \diamond^2 \delta + \dots + c_M e^{\alpha t} \diamond^{M-k} \delta$$

or  $u(t) = e^{\alpha t} \sum_{r=k}^M c_r \diamond^{r-k} \delta$ . Since  $e^{\alpha t} \diamond^{r-k} \delta = L^{r-k}$  for  $k \leq r \leq M$  and  $L$  is defined by (3.2). Thus  $L^{r-k}$  is a singular distribution. It follows that  $u(t)$  is a singular distribution. That complete the proof.  $\square$

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Department of Mathematics, Faculty of Science,  
Chiang Mai University, Chiang Mai 50200, Thailand.