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

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

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Abstract

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

1.1 Introduction

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

1.2 The Time-Dependent Density Matrix (TDDM)

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

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

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

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

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

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

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

the first integral can be done

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

$$\times\int dx''\exp\left(\begin{array}{c} -\frac{1}{2}\frac{(v\cosh v\beta\sin wt - wi\cos wt\sinh v\beta)}{\sin wt\sinh v\beta}(x'')^2 - \frac{wi}{\sin wt}xx'' + \\ \frac{\sin wt\sinh v\beta}{2(v\cosh v\beta\sin wt + wi\cos wt\sinh v\beta)}\left(\frac{v^2\left(x''\right)^2}{\sinh^2 v\beta} - \frac{w^2\left(x'\right)^2}{\sin^2 wt} + \frac{2vwix'x''}{\sinh v\beta\sin wt}\right) \end{array}\right)$$

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

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

1.3 Density of Particles

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

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

where

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

Then the density of particle for distinguishable particles can be calculate

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

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

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

where

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

and

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

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

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

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

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

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

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

using semi-group property

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

Finally,

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

with normalization, from 5

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

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

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

which can be written

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

where

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

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

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

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

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

then

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

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

then, the spatial density distribution can be found by

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

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

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

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

where

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

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

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

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

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

1.3.1 Recursion relation for Partition funtion

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

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

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

then we can find

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

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

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

the next activity can be proceeded from 13 and 11

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

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

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

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

Let call

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

then the formula is

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

Now we can find the recursion relation for the Density

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

from 13

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

then

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

where

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

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

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

Perturbation Theory for the Distinguishable Particles in switching harmonic trap

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

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

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

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

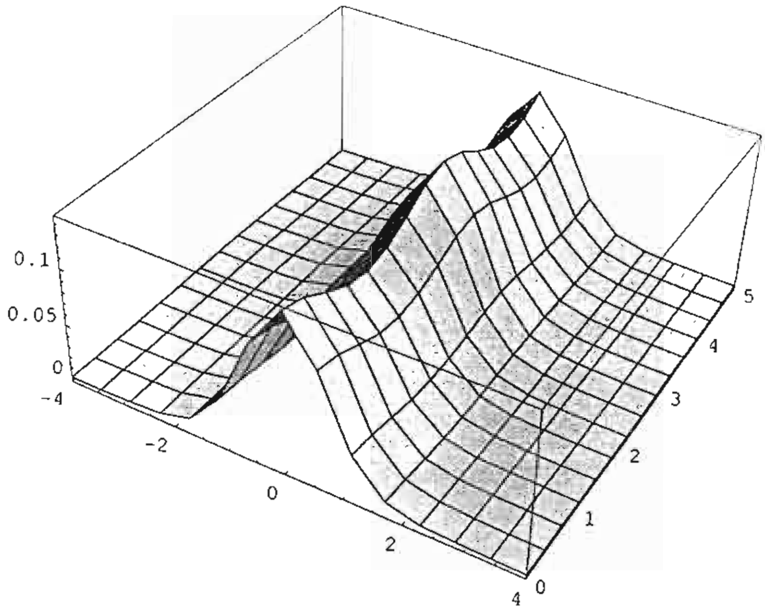

Figure 1: v=1 w=2 N=200

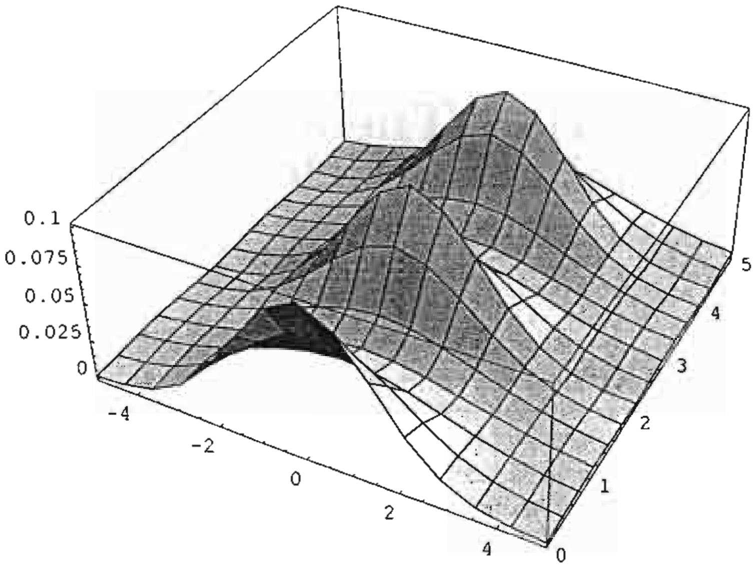

Figure 2: v=1 w=1.1 N=200

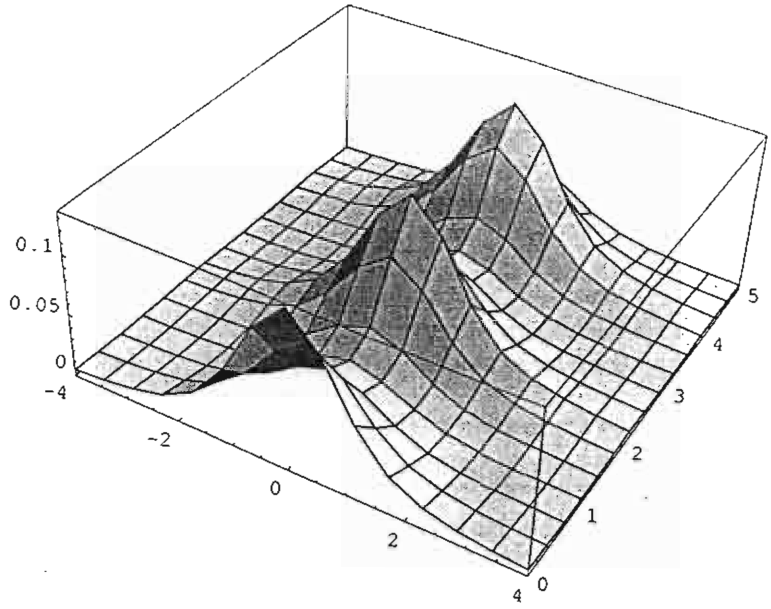

Figure 3: v=1 w=1.01 for N=200

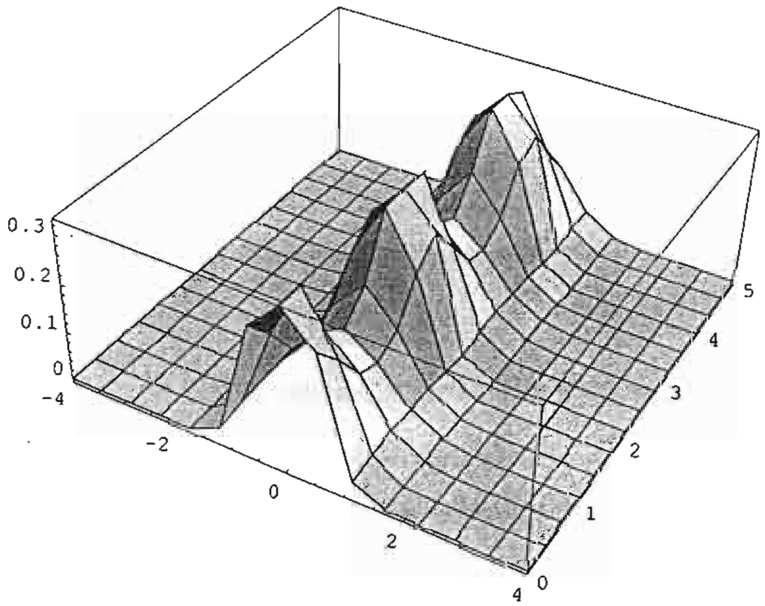

Figure 4: v=1 w=1.5 N=1000

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

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

1.3.2 First Order Approximation

The Time-Dependent Density Matrix

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

To first order perturbation,

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

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

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

$\left[e^{-i\int_0^t dt' H_w} - i\int_0^t dt'\mathcal{T}\left(Ve^{-i\int_0^t dt'' H_w}\right)+...\right]\left[e^{-\int_0^\beta d\tau H_v} - \int_0^\beta d\tau\mathcal{T}\left(Ve^{-\int_0^\beta d\tau' H_v}\right)+...\right]$

$\times\left[e^{i\int_0^t dt' H_w} + i\int_0^t dt'\mathcal{T}\left(Ve^{i\int_0^t dt'' H_w}\right)+...\right]$

$\simeq\left[e^{-itH_w} - i\int_0^t dt' e^{-i(t-t')H_w}Ve^{-it'H_w}\right]\left[e^{-\beta H_v} - \int_0^\beta d\tau e^{-(\beta-\tau)H_v}Ve^{-\tau H_v}+...\right]$

$\times\left[e^{itH_w} + i\int_0^t dt' e^{i(t-t')H_w}Ve^{it'H_w}\right]$

$= e^{-itH_w}e^{-\beta H_v}e^{itH_w} - e^{-itH_w}\int_0^\beta d\tau e^{-(\beta-\tau)H_v}Ve^{-\tau H_v}e^{itH_w} - i\int_0^t dt' e^{-i(t-t')H_w}Ve^{-it'H_w}e^{-\beta H_v}e^{itH_w}$

$+ e^{-itH_w}e^{-\beta H_v}i\int_0^t dt' e^{i(t-t')H_w}Ve^{it'H_w}+...$

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

consider the spatial representation

$\rho(\bar{x}'',t,\beta|\bar{x}')$

$= \langle\bar{x}''|e^{-itH_w}e^{-\beta H_v}e^{itH_w}|\bar{x}'\rangle - \int_0^\beta d\tau\int d\bar{x}\langle\bar{x}''|e^{-itH_w}e^{-(\beta-\tau)H_v}|\bar{x}\rangle V(\bar{x})\langle\bar{x}|e^{-\tau H_v}e^{itH_w}|\bar{x}'\rangle$

$-i\int_0^t dt'\int d\bar{x}\langle\bar{x}''|e^{-i(t-t')H_w}|\bar{x}\rangle V(\bar{x})\langle\bar{x}|e^{-it'H_w}e^{-\beta H_v}e^{itH_w}|\bar{x}'\rangle$

$+i\int_0^t dt'\int d\bar{x}\langle\bar{x}''|e^{-itH_w}e^{-\beta H_v}e^{i(t-t')H_w}|\bar{x}\rangle V(\bar{x})\langle\bar{x}|e^{it'H_w}|\bar{x}'\rangle+...$

$= \rho_\circ(\bar{x}'',t,\beta|\bar{x}') - \int_0^\beta d\tau\int d\bar{x}K_{\frac{1}{2}}(\bar{x}'',t,i(\beta-\tau)|\bar{x})V(\bar{x})K^*_{\frac{1}{2}}(\bar{x}',t,i\tau|\bar{x})$

$-i\int_0^t dt'\int d\bar{x}K_w(\bar{x}'',(t-t')|\bar{x})V(\bar{x})\rho_\circ(\bar{x},t',\beta|\bar{x}') + i\int_0^t dt'\int d\bar{x}\rho_\circ(\bar{x}'',(t-t'),\beta|\bar{x})V(\bar{x})K^*_w(\bar{x}',t$

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

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

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

the terms we need to re-calculate

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

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

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

for the terms

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

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

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

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

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

1.3.3 First perturbation term for distinguishable particles

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

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

We are interested in 2-particles interaction

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

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

then the 1st correction term of density matrix is

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

The Fourier transform of the density (non-normalized)

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

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

consider the term

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

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

where

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

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

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

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

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

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

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

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

1.3.4 Three-point Correlation function for distinguishable particles

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

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

1. $\alpha = i$;

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

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

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

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

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

consider the term

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

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

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

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

2. $\alpha = j$;

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

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

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

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

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

Acknowledgement 3 *The authors (V. Sayakanit) acknowledges the financial support from Thailand Reserach Fund (TRF) and K. Tayanasanti recieved financial support from the Royal Golden Jubilee (RGJ) Ph.D. Program (PHD/00125/2541)*

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

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

ABSTRACT. Replace this text with your own abstract.

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

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12 March 2002

2. INTRODUCTION

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

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

3. Theoretical Model

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

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

Making Fourier Transform we obtain,

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

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

4. Possible Symmetries Consideration

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

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

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

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

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

where[4]

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

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

Substitute these 2 equations into the gap equation

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

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

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

Solving for T_c ,we have the secular equation

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

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

5. Critical Temperature for Pairing

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

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

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

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

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

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

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

for the kinetic energy

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

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

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

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

solving this equation gives

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

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

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

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

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

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

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

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

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

substitute in to the secular equation gives

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$= \frac{4\pi^2 e^{\frac{4}{T_c}\pi\frac{n_B}{m}}}{2\pi^2 e^{\frac{2}{T_c}\pi\frac{n_B}{m}}+3mT_c} \approx \frac{|\mu'|}{2T_c}$$

then the secular equation above is

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

Solution are :

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

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

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

6. Threshold for Boson Pairing

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

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

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

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

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

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

and

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

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

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

where

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

6.0.1. *Low momentum approximation.* The energy reads

$E + 4t\left(\cos P_y + 2\cos\frac{P_y}{2}\cos\frac{\sqrt{3}P_x}{2}\right) \sim$

$E + 4t\left(\left(1 - \frac{1}{2}P_y^2\right) + 2\left(1 - \frac{1}{8}P_y^2\right)\left(1 - \frac{3}{8}P_x^2\right)\right) = 12t + E - 3tP_x^2 - 3tP_y^2 + \ldots$

neglect the term of 4th order.

The fisrt integral $I_\circ$.

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

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

second Integral I_x. $\varphi(\vec{p}) = \left(\frac{1+\sqrt{2}}{\sqrt{3}}\right)\cos P_y + \left(\frac{2-\sqrt{2}}{\sqrt{3}}\right)\cos\frac{P_y}{2}\cos\frac{\sqrt{3}P_x}{2}$
$\sim \left(\frac{1+\sqrt{2}}{\sqrt{3}}\right)\left(1-\frac{1}{2}P_y^2\right) + \left(\frac{2-\sqrt{2}}{\sqrt{3}}\right)\left(1-\frac{1}{8}P_y^2\right)\left(1-\frac{3}{8}P_x^2\right)$
$= \sqrt{3}\left(1-\frac{1}{4}P_x^2+\frac{1}{8}P_x^2\sqrt{2}-\frac{1}{8}P_y^2\sqrt{2}-\frac{1}{4}P_y^2\right)$
$= \sqrt{3}\left(1-\frac{1}{4}\left(1-\frac{\sqrt{2}}{2}1\right)P_x^2-\frac{1}{4}\left(1+\frac{\sqrt{2}}{2}\right)P_y^2\right)$

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

where

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

consider each integral seperately.

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

Let define in the same fashion of [1]

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

then

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

So now we can evaluate I_x

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

For the integral I_{xx}, the factor of $\varphi(\vec{p})^2$ can be approximate to
$\varphi^2(\vec{p}) = \left(\left(\frac{1+\sqrt{2}}{\sqrt{3}}\right)\cos P_y + \left(\frac{2-\sqrt{2}}{\sqrt{3}}\right)\cos\frac{P_y}{2}\cos\frac{\sqrt{3}P_x}{2}\right)^2$
$\sim 3\left(1-\frac{1}{4}\left(1-\frac{\sqrt{2}}{2}1\right)P_x^2 - \frac{1}{4}\left(1+\frac{\sqrt{2}}{2}\right)P_y^2\right)^2$
$= 3\left(1+\frac{1}{2}\left(\frac{\sqrt{2}}{2}-1\right)P_x^2 - \frac{1}{2}\left(1+\frac{\sqrt{2}}{2}\right)P_y^2\right)$
then

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

Summary 1.

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

The Solutions of 6.4 are [1]

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

For $U \to \infty$ then

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

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

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

Then using the equations 6.10, we have

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

Then we can fill in by 6.8

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

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

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

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

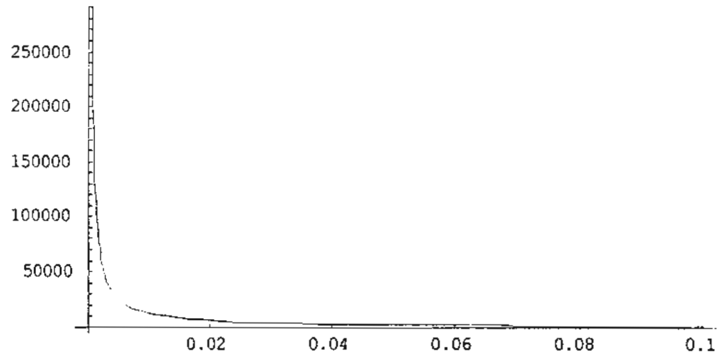
6.1. Bound state consideration. From the T-matrix 6.14 we can see that, for $\frac{J}{t} < \frac{128}{\pi^3}\Omega = \frac{128}{\pi^3}\ln\frac{\tilde{E}}{\tilde{E}-3\pi^2 t}$, the T-matrix is negative which means the two particles bound state occurs and we can evealuate for the bound state energy

$$|\tilde{E}| = \frac{\pi^2 W}{4\left(1-\exp\left(-\frac{\pi^3}{128}\frac{J}{t}\right)\right)} \tag{6.15}$$

where $W = 12t$ the bandwidth of the triangular lattice.
We can consider the relationship

$$\frac{|\tilde{E}|}{t} = \frac{3\pi^2}{1-\exp\left(-\frac{\pi^3}{128}\frac{J}{t}\right)}$$

which can be shown in the picture



where the vertical axe is $\frac{|\tilde{E}|}{t}$ and the horizon one is $\frac{J}{t}$. However, this result must be justified more.

6.2. The Critical Temperature of Pairing from Bethe-Salpeter equation. We have already calculated the critical temperature of $s^* + d_{x^2-y^2}$ pairing by considering from the order parameter or gap equation. Here, by knowing the expression for the T-matrix6.14 we can calculate the critical temperature by another way. By this method we can know the anlytical expression of the temperature which depends on the binding energy. Consider the Bethe-salpeter equation,

$$\Gamma_{s^*+d_{x^2-y^2}} = \frac{T_{s^*+d_{x^2-y^2}}\left(\tilde{E}\right)}{1+T_{s^*+d_{x^2-y^2}}\left(\tilde{E}\right)\int\int\frac{dp_x dp_y}{(2\pi)^2}\frac{\coth\frac{\varepsilon_{\vec{p}}-\mu}{2T}}{2\left(\varepsilon_{\vec{p}}-\mu\right)}} \tag{6.16}$$

$\varepsilon_{\vec{p}} = -2t\left(\left(1-\frac{1}{2}P_y^2\right)+2\left(1-\frac{1}{8}P_y^2\right)\left(1-\frac{3}{8}P_x^2\right)\right) = -6t+\frac{3}{2}tP_x^2+\frac{3}{2}tP_y^2+...$
$\varepsilon_{\vec{p}} \approx -6t+\frac{\vec{p}^2}{2m}$, and $m = \frac{1}{3t}$.
and we absorb $-6t$ to μ by redefine the chemical potential $\tilde{\mu} = \mu + 6t$. The T-matrix which enter in Bethe-Salperter equation have to be evaluated at the binding

energy $\tilde{E} = 2\tilde{\mu}$. and $\tilde{\mu}$ can be determined from the equation for conservation of the number of particles.

$$n = \int\int \frac{dp_x dp_y}{(2\pi)^2} \frac{1}{\exp\left(\frac{\frac{p^2}{2m} - \tilde{\mu}}{2T}\right) - 1} \tag{6.17}$$

which can be solved easily and we use the same crude approximation as in the previous section, we arrive at the solution

$$\tilde{\mu} = -T \exp\left(-\frac{1}{T}\frac{2\pi n_B}{m}\right)$$

And the Temperature can be found from the pole of 6.16

$$1 + T_{s^*+d_{x^2-y^2}}\left(\tilde{E}\right) \int\int \frac{dp_x dp_y}{(2\pi)^2} \frac{\coth \frac{\varepsilon_{\vec{p}} - \mu}{2T}}{2\left(\varepsilon_{\vec{p}} - \mu\right)} = 0 \tag{6.18}$$

which we can use the same calculation procedure as done in the previous section.

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PATH INTEGRAL APPROACH TO A SINGLE POLYMER CHAIN WITH EXCLUDED VOLUME EFFECT

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The effect of a polymer chain with excluded volume representing the long-range interaction between segments along the chain is studied using the Feynman path integral method. The main problem is to calculate the mean square distance, $< R^2 >$, that is

$$< R^2 >= AN^{\nu}$$

where N is the degree of polymerization, ν is a scaling exponent varying from 1-2 for free chain and stiff chain, respectively; and A is a coefficient that depends on the details of the polymer. In the case that the excluded volume interactions are present, $\nu = 6/5$.

The model proposed by Edwards and Singh [1] and Muthukumar and Nickel [2] are employed. Instead of using the idea of an effective step-length technique and the perturbation technique, the idea of Feynman [3] in relation to the polaron problem is used and developed by handling a disordered system. The idea is to model the polymer action as a model of quardatic trial action and consider the differences between the polymer action and the trial action as the first cumulant approximation in one parameter. The variational principle is used to find the optimal values of the variational parameters and the mean square distance is obtained. A comparison between these approaches and effective step-length and perturbation approach will be discussed.

1 Introduction

The theory of the excluded volume effect in a polymer chain is one of the central problems in the field of polymer solution theory representing the effect of the interaction between segments which are far apart along the chain. This interaction is often called the **long-range interaction** in contrast to the **short-range interaction** representing the interaction among a few neighbouring segments.

The polymer excluded volume problem is of the same form and difficulty as the general many body problem, first discussed by Kuhn [4]. The modern development was initiated by Flory [5]. It is recognized that the long-range interaction changes the statistical property of the chain entirely.

The main problem is to calculate the mean square end-to-end distance $\langle R^2 \rangle$, that is

$$< R^2 >= AN^{\nu} \tag{1.1}$$

where the exponent $1<\nu<2$, is to be determined and appears to be solely a function of the dimensionality of space.

Over past decades many attempts have endeavoured to understand the excluded volume effect. One of the theories of the polymer excluded volume problem is the Edwards and Singh's method. A simple method capable of adoption in more complicated problems is developed using the idea of an effective step-length. The mean square value of R^2 is developed as a series which for large L is

$$R^2 = \omega^{\frac{2}{5}} L^{\frac{6}{5}} l^{\frac{2}{5}} (1.12 + 1.05 + 1.03 + \ldots) \tag{1.2}$$

where length $L = Nl$ and ω is the self repulsion.

Another theory is the perturbation which represents a simple derivation of the mean square end-to-end distance $\langle R^2 \rangle$ of a linear-flexible chain as a perturbation series in the dimensionless excluded volume parameter z_d. In an essential way the method used Laplace transforms with respect to the contour length L. The results, to orders six and four in space dimension $d = 3$ and 2, respectively, are

$$\langle R^2 \rangle = Ll[1 + \frac{4}{3} z_3 - 2.075385396\, z_3^2 + 6.296879676\, z_3^3 - 25.05725072\, z_3^4$$
$$+ 116.134785\, z_3^5 - 594.71663\, z_3^6 + \ldots],\ d = 3,$$
$$\langle R^2 \rangle = Ll[1 + \frac{1}{2} z_2 - 0.12154525\, z_2^2 + 0.02663136\, z_2^3 - 0.13223603\, z_2^4 + \ldots],$$
$$d = 2.$$

The purpose of this paper is to calculate the mean square end-to-end distance, employing the model proposed by Edwards [6] and using the idea of Feynman in the polaron problem and one developed by us for handling disordered systems [7]. The idea is to model the system with a trial action containing adjustable, to be determined, parameters. Once the trial action is introduced, the average distribution G can be calculated by expanding in first cumulant approximation about the corresponding trial average distribution G_0. G, approximated by the first cumulant, G_1 can be obtained.

As mentioned above, the parameters should be determined by minimizing the exponent of G_1. However, this procedure leads to a complication because the parameters will depend parametrically on the initial and final position of the polymer chain. To avoid such a complication, a simpler approximation in which only the diagonal contribution of the exponent of G_1 is used in the minimization. This approximation is equivalent to minimizing the free energy. Once the parameters are obtained they will be used to calculate the mean square end-to-end distance.

The outline of the paper is as follows: section 2 is a brief review of an effective step-length technique and the perturbation technique. In section 3, Edwards' model is reviewed. The path integral approach with one parameter model is introduced in section 4. In section 5, the results are discussed and compared with other presentations. Finally, in order to be able to carry out the calculations arising in section 4, an appendix gives a detailed derivation of a characteristic functional corresponding to the trial action $S_0(\omega)$.

2 The Mean Square Distance

2.1 *The Effective Step Length Technique*

The excluded volume problem is a central part of polymer solution theory, the mean-square end-to-end distance agreed on $\langle R^2 \rangle \propto L^\alpha$ where $\alpha = 6/5$ is shown to within one to two percent. Analytic theories based on self consistent fields give α to be exactly 6/5. The chain is considered a locus in space *r(s)*, *s* the arc length, and the random walk constraint is represented by the Wiener measure

$$\exp[-\frac{3}{2l}\int \dot{r}^2(s)ds] \tag{2.1.1}$$

and the interaction

$$\exp\{-\omega\int_0^L\int_0^L \delta[r(s)-r(s')]dsds'\}. \tag{2.1.2}$$

This allows the consideration of $\omega > 0$. The step-length is *l*, and ω has the dimensions of volume. If the symbol $(D(r))$ denotes integration over all paths, then

$$\langle R^2 \rangle = \frac{\int_{r(0)=0}^{r(L)=R} D(r)[r(L)-r(0)]^2 \exp(A)}{\int d^3R \int_{r(0)=0}^{r(L)=R} \exp(A)D(r)}. \tag{2.1.3}$$

Instead it can argued that an effective step-length l_1 be introduced, so that, by definition

$$\langle R^2 \rangle = L l_1 . \tag{2.1.4}$$

Therefore one can write

$$\frac{3}{2l}\int \dot{r}^2 ds + \omega \iint D[r(s) - r(s')] ds ds'$$
$$= \frac{3}{2l_1}\int \dot{r}^2 ds + \{\frac{3}{2}(\frac{1}{l} - \frac{1}{l_1})\int \dot{r}^2 ds + \omega \iint D[r(s) - r(s')] ds ds'\} \tag{2.1.5}$$
$$= \frac{3}{2l_1}\int \dot{r}^2 ds + B \text{, say} \tag{2.1.6}$$
$$= C + B. \tag{2.1.7}$$

Then

$$\langle R^2 \rangle = L l_1 + O(B) + O(B^2) + O(B^3) + \ldots \tag{2.1.8}$$

At this point, choose l_1 so that

$$\langle R^2 \rangle = L l_1$$

so that to first order in B, it gives the equation

$$L l_1^2 (\frac{1}{l} - \frac{1}{l_1}) = 2\sqrt{\frac{6}{\pi^3}}\,\omega \frac{L^{\frac{3}{2}}}{l_1^{\frac{1}{2}}}. \tag{2.1.9}$$

The solution to this equation clearly subsumes perturbation theory, for if ω is small, $l \cong l_1$,

$$\langle R^2 \rangle = L l + 2\sqrt{\frac{6}{\pi^3}}\,\omega L^{\frac{3}{2}} l^{\frac{-1}{2}}. \tag{2.1.10}$$

But for $L^{\frac{1}{2}} > \omega$ there is a Flory type equation with solution

$$l_1 = (2)^{\frac{2}{5}}(\frac{6}{\pi^3})^{\frac{1}{5}}\omega^{\frac{2}{5}} l^{\frac{2}{5}} L^{\frac{6}{5}} \tag{2.1.11}$$

so that

$$\langle R^2 \rangle = (2)^{\frac{2}{5}}(\frac{6}{\pi^3})^{\frac{1}{5}}\omega^{\frac{2}{5}} l^{\frac{2}{5}} L^{\frac{6}{5}}. \tag{2.1.12}$$

To establish the stability of the index α against higher approximations, $\langle R^2 \rangle$ can be written as follows

$$\langle R^2 \rangle = Ll + \frac{A\omega L^{\frac{3}{2}}}{l^{\frac{1}{2}}} + \frac{B\omega^2 L^2}{l^2} + \frac{C\omega^3 L^{\frac{5}{2}}}{l^{\frac{7}{2}}} \tag{2.1.13}$$

where A, B, and C are numbers. Now effective step length l can be introduced to give

$$l = l_1[1 - l_1(\frac{1}{l} - \frac{1}{l_1}) + l_1^2(\frac{1}{l} - \frac{1}{l_1})^2 ...] \tag{2.1.14}$$

Using equation (2.1.14) in (2.1.13) it get to the third in ω

$$\langle R^2 \rangle = Ll_1 - Ll_1^2(\frac{1}{l} - \frac{1}{l_1}) + Ll_1^3(\frac{1}{l} - \frac{1}{l_1})^2 + \frac{A\omega L^{\frac{3}{2}}}{l_1^{\frac{1}{2}}} + \frac{A\omega L^{\frac{3}{2}}}{2} l_1^{\frac{1}{2}}(\frac{1}{l} - \frac{1}{l_1})$$

$$+ \frac{B\omega^2 L^2}{l_1^2} + 2B\omega^2 \frac{l^2}{l_1}(\frac{1}{l} - \frac{1}{l_1}) + \frac{C\omega^3 L^{\frac{5}{2}}}{l^{\frac{7}{2}}} - \tag{2.1.15}$$

Thus the first order approximation gives

$$\alpha = 1.059\omega^{\frac{1}{5}} L^{\frac{1}{10}} l^{\frac{-3}{10}} \tag{2.1.16}$$

$$\langle R^2 \rangle \sim \alpha^2 \simeq Ll_1 = 1.12\omega^{\frac{2}{5}} L^{\frac{6}{5}} l^{\frac{2}{5}}.$$

Now to the second order contained is

$$\alpha = 1.025\omega^{\frac{1}{5}} L^{\frac{1}{10}} l^{\frac{-3}{10}} . \tag{2.1.17}$$

$\langle R^2 \rangle$ still retains the form $\sim \omega^{\frac{2}{5}} L^{\frac{1}{10}} l^{\frac{-3}{10}}$. Now to the third order where

$$\alpha = 1.015\omega^{\frac{1}{5}} L^{\frac{1}{10}} l^{\frac{-3}{10}},$$

$$\langle R^2 \rangle \sim \alpha^2 = 1.03\omega^{\frac{2}{5}} L^{\frac{6}{5}} l^{\frac{2}{5}}. \tag{2.1.18}$$

Finally this can be expressed in a series for $\langle R^2 \rangle$, the additions coming from the order of expansion

$$\langle R^2 \rangle = \omega^{\frac{2}{5}} L^{\frac{6}{5}} l^{\frac{2}{5}} (1.12 + 1.05 + 1.03 + \ldots). \qquad (2.1.19)$$

2.2 The Perturbation Technique

The net effect of the excluded volume interaction between segments of the polymer chain is usually repulsive and leads to an expansion of the chain size. When the excluded volume interaction is very weak, a perturbation theory for the ratio of the mean square end-to-end distance is $\langle R^2 \rangle$ of the chain. Its unperturbed value $\langle R^2 \rangle_0$ can be developed and reduced to a varies in a single dimensionless interaction parameter z_d [8] as

$$\frac{\langle R^2 \rangle}{\langle R^2 \rangle_0} = 1 + C_1 z_d + C_2 z_d^2 + C_3 z_d^3 + \ldots \quad . \qquad (2.2.1)$$

In describing the approach to equation (2.2.1) the equation starts directly with the continuum model and works entirely with the Laplace transform functions $\tilde{G}(E) = \int_0^{\infty} G(L) e^{-EL} dL$, where G(L) are probability functions for a chain's contour length L.

For the standard discrete Gaussian chain model of N+1 segments, the probability distribution function $G_0(R, n)$ can be evaluated and a term of the contour length $L = N\,l$ is given by

$$G_0(R, L) = (\frac{d}{2\pi L l})^{d/2} \exp(-\frac{dR^2}{2Ll}) \quad . \qquad (2.2.2)$$

The mean square end-to-end distance of the Gaussian chain is

$$\langle R^2 \rangle_0 = \int d^d R R^2 G_0(R, L) \Big/ \int d^d R G_0(R, L)$$
$$= Ll. \qquad (2.2.3)$$

When interactions are introduced, the bare distribution will be modified to a non-Gaussian $G(R, L)$ with corresponding characteristic function $\hat{G}(k, L)$ and propagator $\tilde{G}(k, E_0)$. The mean square end-to-end chain distance is given by

$$\langle R^2 \rangle = \int d^d R R^2 G(R,L) \Big/ \int d^d R G(R,L)$$

$$= l \frac{\int \frac{dE_0}{2\pi} e^{E_0 L} [-\frac{2d}{l} \frac{\partial}{\partial k^2} \tilde{G}(k,E_0)]_{k=0}}{\int \frac{dE_0}{2\pi} e^{E_0 L} \tilde{G}(0,E_0)} \ . \quad (2.2.4)$$

This can define a new variable, The so-call "renormalized" energy E by

$$E \equiv E_0 + \sum(0,E_0) \ . \quad (2.2.5)$$

This definition can be reverted order-by-order in perturbation theory to yield $E_0(E)$. If this is defined as

$$\tilde{\Sigma}(k,E) \equiv \tilde{\Sigma}[k,E_0(E)] \ , \quad (2.2.6)$$

then the exact propagator becomes

$$\tilde{G}[k,E_0(E)] = \frac{1}{E + \frac{k^2 l}{2d} + \tilde{\Sigma}(k,E) - \tilde{\Sigma}(0,E)} \ . \quad (2.2.7)$$

These results can be expressed as functions of E and the equation (2.2.4) rewritten as

$$\langle R^2 \rangle = l \int \frac{dE}{2\pi} e^{EL} F_{2(E)} \Big/ \int \frac{dE}{2\pi} e^{EL} F_1(E) \ , \quad (2.2.8)$$

where

$$\begin{aligned} F_1(E) &= E^{-1} J \exp[(E_0 - E)L], \\ F_2(E) &= E^{-1} K F_1(E) L], \end{aligned} \quad (2.2.9)$$

where

$$\begin{aligned} J &= \frac{dE_0}{dE} = 1 - \frac{d}{dE} \tilde{\Sigma}(0,E), \\ K &= 1 + \frac{2d}{l} \frac{\partial}{\partial k^2} \tilde{\Sigma}(k,E)|_{k=0} \ . \end{aligned} \quad (2.2.10)$$

Solving these simultaneous equations in (2.2.9) for F_1 and F_2 , d = 3 is obtained and

$$\langle R^2 \rangle = Ll[1 + \sum_{m=1} C_m z_3^m] \ , \tag{2.2.11}$$

where the coefficients through order m = 6 are

$$z_3 \equiv (\frac{3}{2\pi})^{3/2} \frac{\omega L^{1/2}}{l^{3/2}}, C_1 = 4/3, C_2 = \frac{28\pi}{27} - \frac{16}{3}, C_3 \approx 6.296879676 \ ,$$
$$C_4 \approx -25.05725072 \ , C_5 \approx 116.134785 \ , C_6 \approx -594.71663 \ . \tag{2.2.12}$$

For d = 2, the calculation of $\langle R^2 \rangle$ runs in an exactly analogous manner to the above derivation in d = 3. Then

$$\langle R^2 \rangle = Ll[1 + \sum_{m=1} C_m z_2^m] \tag{2.2.13}$$

where

$$z_2 \equiv \frac{\omega L}{\pi l}, C_1 = 1/2, C_2 = -0.1215452 \ ,$$
$$C_3 = 0.0266313 \ , C_4 = -0.13223603 \ . \tag{2.2.14}$$

3 Edwards' Model

In an ideal polymer, there is only a short-range interaction and the action can be written as

$$S = \frac{3}{2l^2} \int_0^N d\tau \dot{R}^2(\tau) \tag{3.1}$$

where l is the effective bond length representing the short-range interaction, and $R(\tau)$ is the position of segment τ of the polymer.

Since there are many effects in real polymers, the long-range interaction is quite complicated: steric effects, Van der Waals attraction, and solvent molecules effect. However, for the large-length scale concerned, the details of the interaction can be omitted. Thus the interaction between the polymer segments τ and σ can be expressed as

$$k_B T v(R_\tau - R_\sigma) \ .$$

This can be approximated even further by a delta function

$$v k_B T \delta(R_\tau - R_\sigma) ,$$

where v is the excluded volume which represents the long-range interaction, and has the dimension of volume.

The total interaction energy is thus written as

$$U_1 = \frac{v}{2} k_B T \int_0^N \int_0^N d\tau d\sigma \delta(R(\tau) - R(\sigma)) \tag{3.2}$$

using the local concentration of the segments

$$c(r) = \int_0^N d\tau \delta(r - R(\tau)) \ . \tag{3.3}$$

Thus, equation (3.2) may be rewritten

$$U_1 = \int d r \frac{1}{2} v k_B T c(r)^2 \ . \tag{3.4}$$

This statement indicates that equation (3.2) is the first term in the virial expansion of the free energy with respect to the local concentration $c(r)$. Now if the interaction equation (3.2) is taken into account, the action becomes

$$S = \frac{3}{2l^2} \int_0^N d\tau \dot{R}^2(\tau) + \frac{v}{2} \int_0^N \int_0^N d\tau d\sigma \delta(R(\tau) - R(\sigma)) \ . \tag{3.5}$$

The second term accounts for excluded volume interactions between segments of the polymer. The probability distribution of the end-to-end distance is given by

$$G(R_2, R_1; N) = \int_{R_1}^{R_2} D[R(\tau)] e^{-S} \ . \tag{3.6}$$

4 Path Integral Approach

In this section, we apply the idea of Feynman, developed for the polaron problem, and Sa-yakanit[9], applied to disorder system, to polymer problem . This idea is to model the system with a model trial action which can be solved exactly for one parameter model.

The Edwards action is exactly solvable only in the limit, v = 0, where no excluded volume interactions are presented. In this case, the polymer exhibits Gaussian statistics. If v is not zero, the model is no longer exactly solvable;

However, this problem is similar to a polaron problem, which can be solved by path integral and variation method, by introducing the trial action $S_0(\omega)$.

$$S_0(\omega)=\frac{m}{2}\int_0^N d\tau\,\dot{R}^2(\tau)+\frac{m\omega^2}{4N}\int_0^N\int_0^N d\tau d\sigma\,(R(\tau)-R(\sigma))^2 \tag{4.1}$$

where $m = 3/l^2$ and ω is a parameter.

Once the trial action $S_0(\omega)$ has been introduced, it is possible to find the average distribution which, from equation (3.6) can be rewritten as

$$G(R_2,R_1;N) = G_0(R_2,R_1;N,\omega) < \exp[S_0(\omega)-S] >_{S_0(\omega)}\ , \tag{4.2}$$

where the trial distribution $G_0(R_2,R_1;N,\omega)$ is defined by

$$G_0(R_2,R_1;N) = \int_{R_1}^{R_2} D[R(\tau)]e^{-S_0(\omega)}\ , \tag{4.3}$$

and the average $< x >_{S_0(\omega)}$ is defined as

$$< X >_{S_0(\omega)} = \frac{\int_0^N D[R(\tau)]Xe^{-S_0(\omega)}}{\int_0^N D[R(\tau)]e^{-S_0(\omega)}}\ . \tag{4.4}$$

Approximating equation (4.2) by the first cumulant, we get

$$G_1(R_2,R_1;N) = G_0(R_2,R_1;N,\omega) < \exp[S_0(\omega)-S] >_{S_0(\omega)}\ . \tag{4.5}$$

To obtain $G_1(R_2,R_1;N)$, find $G_0(R_2,R_1;N)$ and the average. Firstly, consider the average $< S_0(\omega)-S >_{S_0(\omega)}$. Since the first term in S and $S_0(\omega)$ always cancel each other, this denotes $< S >_{S_0(\omega)}$ and $< S_0(\omega) >_{S_0(\omega)}$ for convenience as the averages of the second term respectively. The average of $< S >_{S_0(\omega)}$ can be evaluated by making a Fourier decomposition of $\delta(R(\tau)-R(\sigma))$. Thus,

$$\langle S\rangle_{S_0(\omega)} = \frac{v}{2}\int_0^N\int_0^N d\tau d\sigma\left(\frac{1}{2\pi}\right)^3\int dk\,\langle \exp[ik.(R(\tau)-R(\sigma))]\rangle_{S_0(\omega)}\ . \tag{4.6}$$

The average on the right-hand side of equation (4.6) can be expanded in cumulants, and because $S_0(\omega)$ is quadratic, only the first two cumulants are non-zero [10]. Equation (4.6) becomes

$$\langle S\rangle_{S_0(\omega)} = \frac{V}{2}\int_0^N\int_0^N d\tau d\sigma\left(\frac{1}{2\pi}\right)^3 \int dk \exp(x_1 + x_2) \ , \tag{4.7}$$

where

$$x_1 = ik.\langle R(\tau) - R(\sigma)\rangle_{S_0(\omega)} \ , \tag{4.8}$$

and

$$x_2 = \frac{-k^2}{2}\left[\frac{1}{3}\left\langle (R(\tau) - R(\sigma))^2\right\rangle_{S_0(\omega)} - \langle R(\tau) - R(\sigma)\rangle_{S_0(\omega)}\right] \ . \tag{4.9}$$

Note that the second term inside the square brackets of equation (4.9) represents only one component of the coordinates. Performing the k-integration results in

$$\langle S\rangle_{S_0(\omega)} = \frac{V}{2}\int_0^N\int_0^N d\tau d\sigma\left(\frac{1}{2\pi}\right)^3 A^{-3/2} \exp\left(\frac{-B^2}{4A}\right) \tag{4.10}$$

where

$$A = \frac{1}{2}\left[\frac{1}{3}\left\langle (R(\tau) - R(\sigma))^2\right\rangle_{S_0(\omega)} - \langle R(\tau) - R(\sigma)\rangle_{S_0(\omega)}\right] \tag{4.11}$$

and

$$B = i\langle R(\tau) - R(\sigma)\rangle_{S_0(\omega)} \ . \tag{4.12}$$

Next we consider the average of $< S_0(\omega) >_{S_0(\omega)}$ which is easily written as

$$\langle S_0(\omega)\rangle_{S_0(\omega)} = \frac{m\omega^2}{4N}\int_0^N\int_0^N d\tau d\sigma\left\langle (R(\tau) - R(\sigma))^2\right\rangle_{S_0(\omega)} \ . \tag{4.13}$$

4.1 *The Characteristic Functional*

From equations (4.10) and (4.13) it can be seen that the average $< S_0(\omega) - S >_{S_0(\omega)}$ can be expressed solely in terms of the following averages: $< R(\tau) >_{S_0(\omega)}$ and $< R(\tau)R(\sigma) >_{S_0(\omega)}$. Such averages can be obtained from a characteristic functional of

$<\exp(\int_0^N d\tau f(\tau)R(\tau))>_{S_0(\omega)}$. From Feynman and Hibbs, the characteristic functional can be expressed as

$$<\exp(\int_0^N d\tau f(\tau)R(\tau))>_{S_0(\omega)}=\exp(-[S'_{0,cl}(R_2-R_1;N,\omega)-S_{0,cl}(R_2-R_1;N,\omega)]) \quad , \tag{4.1.1}$$

where $S'_{0,cl}(R_2-R_1;N,\omega)$ and $S_{0,cl}(R_2-R_1;N,\omega)$ are two classical actions which we have derived from the calculation in the Appendix. Once the classical action $S'_{0,cl}(R_2-R_1;N,\omega)$ is obtained, we can differentiate expression (4.1.1) with respect to $f(\tau)$ to obtain

$$\begin{aligned}\langle R(\tau)\rangle_{S_0(\omega)} &= -\frac{\delta S'_{0,cl}(R_2-R_1;N,\omega)}{\delta f(\tau)}\Big|_{f(\tau)=0} \\ &= \frac{m\omega}{2\sinh\omega N}\Bigg[\frac{2R_2}{m\omega}\left(\sinh\omega\tau+2\sinh\frac{\omega N}{2}\sinh\frac{\omega(N-\tau)}{2}\sinh\frac{\omega\tau}{2}\right) \\ &\quad+\frac{2R_1}{m\omega}\left(\sinh\omega(N-\tau)+2\sinh\frac{\omega N}{2}\sinh\frac{\omega(N-\tau)}{2}\sinh\frac{\omega\tau}{2}\right)\Bigg]\end{aligned} \tag{4.1.2}$$

where the symbol $|_{f(\tau)=0}$ implies that after the differentiation, $f(\tau)=0$ must be set. Continuing the differentiation,

$$\begin{aligned}\langle R(\tau)R(\sigma)\rangle_{S_0(\omega)} = [&-\frac{\delta^2 S'_{0,cl}(R_2-R_1;N,\omega)}{\delta f(\tau)\delta f(\sigma)} \\ &+\frac{\delta S'_{0,cl}(R_2-R_1;N,\omega)}{\delta f(\tau)}.\frac{\delta S'_{0,cl}(R_2-R_1;N,\omega)}{\delta f(\sigma)}]\Big|_{f(\tau)=0} .\end{aligned} \tag{4.1.3}$$

Set $\sigma=\tau$ in equation(4.1.3) to obtain

$$\left\langle R^2(\tau)\right\rangle_{s,(\omega)} = \frac{3}{m\omega}\left\{\frac{\sinh\omega(N-\tau)\sinh\omega\tau}{\sinh\omega N} + \frac{4\sinh^2\frac{\omega}{2}(N-\tau)\sinh^2\frac{\omega}{2}\tau}{\sinh\omega N}\right\}$$
$$+\left[R_2\left(\frac{\sinh\omega\tau}{\sinh\omega N} + \frac{2\sinh\frac{\omega N}{2}\sinh\frac{\omega(N-\tau)}{2}\sinh\frac{\omega\tau}{2}}{\sinh\omega N}\right)\right.$$
$$\left.+R_1\left(\frac{\sinh\omega(N-\tau)}{\sinh\omega N} + \frac{2\sinh\frac{\omega N}{2}\sinh\frac{\omega(N-\tau)}{2}\sinh\frac{\omega\tau}{2}}{\sinh\omega N}\right)\right]^2 . \tag{4.1.4}$$

Equation (4.1.4) is the mean square end-to-end distance of the polymer. This method is more general than another methods because the mean square can be found at any point along the polymer chain.

Using equations (4.1.2) and (4.1.3) and performing the integration in equation (4.13) the following is obtained:

$$\left\langle S_0(\omega)\right\rangle_{s,(\omega)} = \frac{3}{2}\left(\frac{\omega N}{2}\coth\frac{\omega N}{2} - 1\right)$$
$$+\frac{m}{2}\left[\frac{\omega N}{2}\coth\frac{\omega N}{2} - \left(\frac{\omega N}{2}\operatorname{cosech}\frac{\omega N}{2}\right)^2\right]\frac{(R_2-R_1)^2}{2N} . \tag{4.1.5}$$

Collecting the above results, the following is obtained:

$$G_1(R_2-R_1;N,\omega) = \left(\frac{3}{2\pi N l^2}\right)^{3/2}\left(\frac{\omega N}{2\sinh\frac{\omega N}{2}}\right)^3$$
$$\exp\Big[\left(\frac{-3\omega}{4l^2}\right)(R_2-R_1)^2\left(\frac{1}{2}\coth\frac{\omega N}{2} + \frac{\omega N}{4}\operatorname{cosech}^2\frac{\omega N}{2}\right)$$
$$-\frac{3}{2} + \frac{3\omega N}{4}\coth\frac{\omega N}{2}$$
$$-\frac{v}{2}\int_0^N\int_0^N d\tau d\sigma\left(\frac{1}{4\pi}\right)^{3/2} A^{-3/2}\exp\left(\frac{-B^2}{4A}\right) , \tag{4.1.6}$$

where we find for $\tau > \sigma$

$$A = \frac{\sinh\frac{\omega(\tau-\sigma)}{2}\sinh\frac{\omega(N-(\tau-\sigma))}{2}}{m\omega\sinh\frac{\omega N}{2}} \tag{4.1.7}$$

and

$$B = \frac{i.\sinh\frac{\omega(\tau-\sigma)}{2}\cosh\frac{\omega(N-(\tau+\sigma))}{2}}{\sinh\frac{\omega N}{2}}.(R_2 - R_1). \tag{4.1.8}$$

$G_1(R_2 - R_1; N, \omega)$ is the average distribution in the first cumulant. To determine $<R^2(\tau)>$, ω must be found first. Three cases are considered:

Case I ($\nu = 0$ and $\omega = 0$)

This case is the free polymer chain or the chain without excluded volume effect. $\frac{\partial \ln G_1(R_2, R_1; N, \omega)}{\partial R_2} = 0$ was calculated, This approximation is equivalent to minimizing the free energy, then $R_2 = R_1$ was obtained. If one end of the polymer chain at the origin ($R_1 = 0$) is fixed and taken to the limit $\omega \to 0$ in equation (4.1.4), then

$$\langle R^2(\tau)\rangle \approx \frac{l^2(N-\tau)\tau}{N}. \tag{4.1.9}$$

Equation (4.1.9) represents the mean square distance at any points along the chain without volume effect–free polymer chain. This result corresponds to the experiment and another methods, but is more general as can be seen for $N \to \infty$:

$$\langle R^2(\tau)\rangle \approx l^2\tau .$$

Cases II and III

In cases II and III, the variational method was used by minimizing the diagonal contribution of the exponent of $G_1(R_2 - R_1; N, \omega)$. This approximation is equivalent to minimizing the free energy:

$$\frac{\partial \ln \mathrm{Tr} G_1(R_2, R_1; N, \omega)}{\partial \omega} = 0. \tag{4.1.10}$$

Thus

$$\left(1-\frac{\omega N}{2}\coth\frac{\omega N}{2}\right)$$

$$+\frac{1}{2}\left(\left(\frac{\omega N}{2}\coth\frac{\omega N}{2}\right)-\left(\frac{\omega N}{2}\operatorname{cosech}\frac{\omega N}{2}\right)^{2}\right)=\frac{vN}{4m}\left(\frac{1}{4\pi}\right)^{3/2}\int_0^N dxA^{-5/2}$$

$$\left[\frac{\sinh\frac{\omega x}{2}\sinh\frac{\omega(N-x)}{2}}{\omega\sinh\frac{\omega N}{2}}-\frac{N\sinh^{2}\frac{\omega x}{2}}{2\sinh^{2}\frac{\omega N}{2}}\right.$$

$$\left.-\frac{x\sinh\frac{\omega(N-2x)}{2}}{2\sinh\frac{\omega N}{2}}\right], \quad (4.1.11)$$

where $x = \tau - \sigma$ and $\tau > \sigma$. Equations (4.1.6) and (4.1.11) represent a complete determination of $G_1(R_2 - R_1; N, \omega)$; however, they can not be solved exactly.

In Case II (ω is small and v is not zero):

Equation (4.1.11) was approximated as

$$1-\frac{\omega N}{4}-\frac{(\omega N)^{2}e^{-\omega N}}{2}=\frac{1}{4}\left(\frac{m}{2\pi}\right)^{3/2} vN\omega^{1/2}(1+\omega N)(1-e^{-\omega N}). \quad (4.1.12)$$

By substituting equation (4.1.12) in equation (4.1.4) the following was obtaind:

$$\langle R^{2}\rangle = Nl^{2}\left[\frac{1}{4}+\frac{7vm^{3/2}N^{1/2}}{20\sqrt{2}\pi^{3/2}}-\frac{273m^{3}v^{2}N}{2000\pi^{3}}+\ldots\right]. \quad (4.1.13)$$

In Case III (ω is large and v is not zero):

Equation (4.1.11) can be expressed in asymptotic form as

$$\left(1-\frac{\omega N}{2}\right)+\frac{\omega N}{4}=\frac{vN}{4m}\left(\frac{1}{4\pi}\right)^{3/2}\int_0^N dx\left(\frac{1}{2m\omega}\right)^{-5/2}\left(\frac{1}{2\omega}\right)$$

$$1-\frac{\omega N}{4}=\left(\frac{vN^{2}}{4}\right)\left(\frac{m}{2\pi}\right)^{3/2}\omega^{3/2}$$

$$\omega=\left(\frac{2\pi}{m}\right)\left(\frac{4}{v}\right)^{2/3}N^{-4/3}\left(1-\frac{\omega N}{4}\right)^{2/3}. \quad (4.1.14)$$

Asymptotically substituting equation (4.1.14) into (4.1.4) to obtain

$$\langle R^2\rangle \approx \left(\frac{3}{2\pi}\right)\left(\frac{v}{4}\right)^{2/3} N^{4/3}. \qquad (4.1.15$$

5 Discussion and Conclusions

The paper studied the polymer-excluded volume employing the Feynman pat integral method with the model proposed by Edwards. The calculation that follow is developed by us for handling the disorder system. The average mean squar displacement at any length in the polymer is obtained. Therefore the result is mor general than other methods where only the end-to-end point is calculated. In order t be able to appreciate the result of these calculations see Table 1.

Table 1.

Model Case	Perturbation	Edwards	Our method
Free chain	Nl^2	Nl^2	$\frac{l^2(N-\tau)\tau}{N}$
Weak interaction	$Nl^2\left(1+\frac{4}{3}\left(\frac{3}{2\pi l}\right)^{\frac{3}{2}}\omega L^{\frac{1}{2}}\right)$	-----	$\frac{Nl^2}{4}$
Strong interaction	------	$1.12\omega^{\frac{2}{5}}N^{\frac{6}{5}}l^{\frac{8}{5}}$	$\left(\frac{3}{2\pi}\right)\left(\frac{v}{4}\right)^{\frac{2}{3}}N^{\frac{4}{3}}$

Table 1: Present results are compared with the perturbation method and th method developed by Edwards. From the table for free chain all approaches lead t Nl^2. Note that since the present results give detailed information along the chain Therefore $N\to\infty$, $\frac{(N-\tau)\tau}{N}\to N$ and the present results will coincide with the fre chain. For weak interaction the present results differ from the perturbation by a factor of 1/4 . This is due to our approximation by using harmonic approximation. It is well known that a harmonic approximation always leads to unphysical results for weak ω. Finally, for strong interaction the present result is $N^{4/3}$ instead of $N^{6/5}$ as

obtained by Edwards. It is noticeable that the harmonic approximation is also not very good for strong interaction. The reason is that a harmonic trial action cannot model the delta function in this excluded volume problem because the delta function has a bounded state at minus infinity. If our excluded volume has a finite range then the harmonic trial action will be able to model the long-range problem. Future research will consider more of this problem. Although the use of a harmonic trial action does not correctly produce the weak and strong coupling in the exponent, it does give the prefactor A correctly which is important for calculating the magnitude of the mean square displacement. This result can be recognized by noticing that

$$< R^2 >= AN^{\nu} .$$

Then the exponent can be obtained by plotting ν againt $\ln\left[\frac{\langle R^2\rangle}{l^2}\right]/\ln[N]$ for large N. The $<R^2>$ can be taken from equation (4.1.4) and the result is given in Fig. 1.

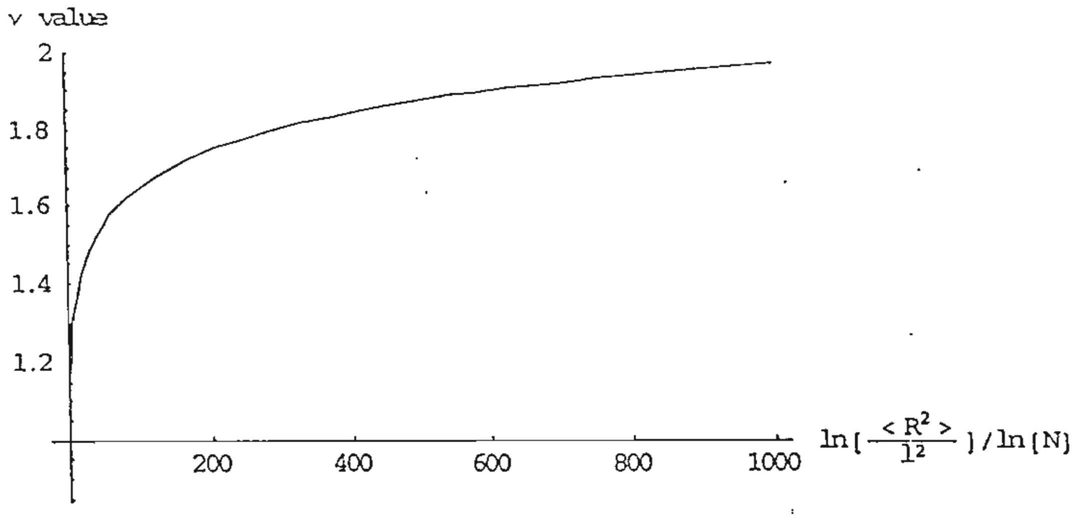

Figure 1.

The advantage of the variational method is that the mean square displacement of the polymer chain with excluded volume for any coupling strength and fluctuation along the length of the polymer can be obtained. The intermediate strength is shown graphically in Fig. 1.

Finally, this method can be generalized to two parameters as in the case of polaron.

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7 Appendix

In order to evaluate the averages of $<\mathrm{R}(\tau)>_{S_0(\omega)}$ and $<\mathrm{R}(\tau)\mathrm{R}(\sigma)>_{S_0(\omega)}$, it is nescessary to establish a characteristic functional, as

$$<\exp\left(\int_0^N d\tau \mathrm{f}(\tau)\mathrm{R}(\tau)\right)>_{S_0(\omega)}=\frac{\int_0^N D[\mathrm{R}(\tau)]\exp(-S_0(\omega)+\int_0^N d\tau \mathrm{f}(\tau).\mathrm{R}(\tau))}{\int_0^N D[\mathrm{R}(\tau)]\exp(-S_0(\omega))} \qquad \text{(A1)}$$

where $\mathrm{f}(\tau)$ is any arbitray function of time, equation (A1) suggests that if the trial action $S_0(\omega)$ is quadratic, then the action of $S_0^{'}(\omega)=S_0(\omega)-\int_0^N d\tau \mathrm{f}(\tau)\mathrm{R}(\tau)$. Using Feynman and Hipps, the path integral of equation (A1) can be carried out exactly as

$$<\exp(\int_0^N d\tau \mathrm{f}(\tau)\mathrm{R}(\tau))>_{S_0(\omega)}=\exp\left(-\left[S_{0,cl}^{'}(\mathrm{R}_2-\mathrm{R}_1;N,\omega)-S_{0,cl}(\mathrm{R}_2-\mathrm{R}_1;N,\omega)\right]\right) \qquad \text{(A2)}$$

where $S_{0,cl}^{'}(\mathrm{R}_2-\mathrm{R}_1;N,\omega)$ and $S_{0,cl}(\mathrm{R}_2-\mathrm{R}_1;N,\omega)$ are the corresponding classical actions of $S_{0,cl}^{'}(\omega)$ and $S_{0,cl}(\omega)$. When the classical action $S_{0,cl}^{'}(\mathrm{R}_2-\mathrm{R}_1;N,\omega)$ is obtained, the classical action $S_{0,cl}(\mathrm{R}_2-\mathrm{R}_1;N,\omega)$ can be obtained form it by setting $\mathrm{f}(\tau)=0$.

To obtain the classical action $S_{0,cl}^{'}(\mathrm{R}_2-\mathrm{R}_1;N,\omega)$ a variation is required for $S_{0,cl}^{'}(\omega)$ to obtain the equation

$$\frac{d^2\mathrm{R}_c(\tau)}{d\tau^2}-\frac{\omega^2}{N}\int_0^N d\sigma(\mathrm{R}_c(\tau)-\mathrm{R}_c(\sigma))=\frac{\mathrm{f}(\tau)}{m}. \tag{A3}$$

This equation may be rewritten in the form

$$\frac{d^2\mathrm{R}_c(\tau)}{d\tau^2}-\omega^2\mathrm{R}_c(\tau)=-\frac{\omega^2}{N}\int_0^N d\sigma\mathrm{R}_c(\sigma)-\frac{\mathrm{f}(\tau)}{m}. \tag{A4}$$

By introducing a Green Function

$$\left(\frac{d^2}{d\tau}-\omega^2\right)g(\tau,\sigma)=\delta(\tau-\sigma) \tag{A5}$$

where

$$g(\tau,\sigma)=-\left[\frac{\sinh\omega(N-\tau)\sinh\omega\sigma H(\tau-\sigma)+\sinh\omega(N-\sigma)\sinh\omega\tau H(\sigma-\tau)}{\omega\sinh\omega N}\right], \tag{A6}$$

with H denoting the Heviside step function, then the general solution of equation (A5) with the boundary condition $\mathrm{R}(0)=\mathrm{R}_1$ and $\mathrm{R}(N)=\mathrm{R}_2$ can be written as

$$\mathrm{R}_c(\tau)=\frac{[\mathrm{R}_2\sinh\omega\tau+\mathrm{R}_1\sinh\omega(N-\tau)]}{\sinh\omega N} -\int_0^N\left[\frac{\mathrm{f}(\sigma)}{m}+\frac{\omega^2}{N}\int_0^N R(\sigma)d\sigma\right]g(\tau,\sigma)d\sigma \tag{A7}$$

This equation (A7) is an integral equation which can be solved. The solution is

$$\mathrm{R}_c(\tau)=\frac{[\mathrm{R}_2\sinh\omega\tau+\mathrm{R}_1\sinh\omega(N-\tau)]}{\sinh\omega N}-\int_0^N\frac{\mathrm{f}(\sigma)}{m}g(\tau,\sigma)d\sigma + \frac{(\mathrm{R}_1+\mathrm{R}_1)\sinh\frac{\omega\tau}{2}\sinh\frac{\omega(N-\tau)}{2}}{\cosh\frac{\omega N}{2}}$$

$$+\frac{4\sinh\frac{\omega\tau}{2}\sinh\frac{\omega(N-\tau)}{2}\int_0^N \mathbf{f}(\sigma)\sinh\frac{\omega\sigma}{2}\sinh\frac{\omega(N-\sigma)}{2}d\sigma}{m\omega\sinh\omega N} \tag{A8}$$

The classical action of $S'_{0,cl}(\mathrm{R}_2-\mathrm{R}_1;N,\omega)$ is simply obtained by substituting R_c into the expression

$$S'_0(\mathrm{R}_2-\mathrm{R}_1;\omega,N)=\frac{m}{2}\int_0^N d\tau\,\dot{\mathrm{R}}_c^2(\tau)+\frac{m\omega^2}{4N}\int_0^N\int_0^N d\tau d\sigma(\mathrm{R}_c(\tau)-\mathrm{R}_c(\sigma))^2$$
$$-\int_0^N d\tau \mathbf{f}(\tau)\mathrm{R}_c(\tau)$$
$$=\frac{m}{2}\left[\dot{\mathrm{R}}_c(N)\mathrm{R}_c(N)-\dot{\mathrm{R}}_c(0)\mathrm{R}_c(0)\right] \tag{A9}$$

to give

$$S'_0(\mathrm{R}_2-\mathrm{R}_1;\omega)=\frac{m\omega}{4}\coth\frac{\omega N}{2}|\mathrm{R}_2-\mathrm{R}_1|^2$$
$$-\frac{m\omega}{2\sinh\omega N}[\frac{2\mathrm{R}_2}{m\omega}\int_0^N d\tau\mathbf{f}(\tau)(\sinh\frac{\omega\tau}{2}$$
$$+2\sinh\frac{\omega N}{2}\sinh\frac{\omega\tau}{2}\sinh\frac{\omega(N-\tau)}{2})$$
$$+\frac{2\mathrm{R}_1}{m\omega}\int_0^N d\tau\mathbf{f}(\tau)(\sinh\frac{\omega(N-\tau)}{2}$$
$$+2\sinh\frac{\omega N}{2}\sinh\frac{\omega\tau}{2}\sinh\frac{\omega(N-\tau)}{2})$$
$$+\frac{2}{m^2\omega^2}\int_0^N\int_0^\tau d\tau d\sigma\mathbf{f}(\tau)\mathbf{f}(\sigma)(\sinh\omega(N-\tau)\sinh\omega\sigma$$
$$+4\sinh\frac{\omega\tau}{2}\sinh\frac{\omega(N-\tau)}{2}\sinh\frac{\omega\sigma}{2}\sinh\frac{\omega(N-\sigma)}{2})] \tag{A10}$$

The classical action $S_{0,cl}(\mathrm{R}_2-\mathrm{R}_1;N,\omega)$ is then obtained by setting $\mathrm{f}(\tau)=0$ in equation (A10):

$$S_0(\mathrm{R}_2-\mathrm{R}_1;\omega)=\frac{m\omega}{4}\coth\frac{\omega N}{2}\left|\mathrm{R}_2-\mathrm{R}_1\right|^2. \tag{A11}$$

Next, to evaluate the trial propagator $G_0(\mathrm{R}_1,\mathrm{R}_2;N,\omega)$, the trial action is rewritten as $S_0(\omega)$ in the form

$$S_0(\omega)=S_0(HP)-\frac{m\omega}{2N}\left(\int_0^N d\tau\mathrm{R}(\tau)\right)^2 \tag{A12}$$

where $S_0(HP)$ is the simple harmonic potential action as shown in

$$S_0(HP)=\int_0^N d\tau\frac{m}{2}\left(\dot{\mathrm{R}}^2(\tau)+\omega^2\mathrm{R}^2(\tau)\right). \tag{A13}$$

The second term of equation (A12) can be converted to an integral form by the identity

$$\exp\left[\frac{m\omega^2}{2N}\left(\int_0^N d\tau\mathrm{R}(\tau)\right)^2\right]=\left(\frac{N}{2\pi m\omega^2}\right)^{3/2}\int d\mathrm{f}\exp\left(\frac{-N\mathrm{f}^2}{2m\omega^2}-\int_0^N d\tau\mathrm{R}(\tau)\mathrm{f}\right). \tag{A14}$$

Form equations (A12) and (A14), it can be found that the propagator G_0 can be expressed as

$$G_0(\mathrm{R}_2,\mathrm{R}_1;N,\omega)=\left(\frac{N}{2\pi m\omega^2}\right)^{3/2}\int_{\mathrm{R}_1}^{\mathrm{R}_2}D[\mathrm{R}(\tau)]\int d\mathrm{f}\exp\left[-(S_0(HP)+\frac{N\mathrm{f}^2}{2m\omega^2}+\int_0^N d\tau\mathrm{R}(\tau)\mathrm{f})\right]. \tag{A15}$$

Changing the order of integration, (A15) becomes

$$G_0(\mathrm{R}_2,\mathrm{R}_1;N,\omega)=\left(\frac{N}{2\pi m\omega^2}\right)^{3/2}\int df\,\exp\left[-\frac{N\mathrm{f}^2}{2m\omega^2}\right]G_{\mathrm{f}}(\mathrm{R}_2,\mathrm{R}_1;N,\mathrm{f}) \tag{A16}$$

where

$$G_{\mathrm{f}}(\mathrm{R}_2,\mathrm{R}_1;N,\mathrm{f})=\int_{\mathrm{R}_1}^{\mathrm{R}_2}D[\mathrm{R}(\tau)]\exp\left[-(S_0(HP)+\int_0^N d\tau \mathrm{R}(\tau)\mathrm{f})\right]. \tag{A17}$$

The propagator (A17) is the force hamonic oscillator propagator with a constant external force f, which is

$$\begin{aligned}G_{\mathrm{f}}(\mathrm{R}_2,\mathrm{R}_1;N,\mathrm{f})=&\left(\frac{m\omega}{2\pi\sinh\omega N}\right)^{3/2}\exp[-(\frac{m\omega}{4}(\coth\frac{\omega N}{2}|\mathrm{R}_2-\mathrm{R}_1|^2\\&+\tanh\frac{\omega N}{2}(\mathrm{R}_2+\mathrm{R}_1)^2)+\frac{1}{\omega}\tanh\frac{\omega N}{2}(\mathrm{R}_2+\mathrm{R}_1)\mathrm{f}\\&+(\frac{1}{m\omega^3}\tanh\frac{\omega N}{2}-\frac{N\mathrm{f}^2}{2m\omega^2}))]\ .\end{aligned} \tag{A18}$$

Substituting (A18) into (A16), and performing the f-integration, equation (A19) is obtained:

$$G_0(\mathrm{R}_2,\mathrm{R}_1;N,\omega)=\left(\frac{m}{2\pi N}\right)^{3/2}\left(\frac{\omega N}{2\sinh\frac{\omega N}{2}}\right)^3\exp[-\frac{m\omega}{4}\coth\frac{\omega N}{2}|\mathrm{R}_2-\mathrm{R}_1|^2] \tag{A1}$$

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ฟังก์ชันการกระจายแบบคู่ของโลหะเหลวไฮโดรเจน ถูกคำนวณออกมาภายใต้เงื่อนไข ความหนาแน่น ความดัน และ อุณหภูมิ ต่าง ๆ โดยวิธีการแก้สมการของ Ornstein – Zernike อาศัยการประมาณแบบ Percus – Yevick ในกรณีที่ศักย์ของอะตอมเป็นแบบทรงกลมแกร่ง ผลเฉลยที่ได้เป็นฟังก์ชันที่ขึ้นอยู่กับรัศมีทรงกลม ซึ่งสามารถคำนวณได้จากสมการสถานะเมื่อทราบ ความหนาแน่น ความดัน และ อุณหภูมิ ด้วยวิธีการเดียวกันนี้เรายังคำนวณค่าปัจจัยโครงสร้าง $S(k)$ ซึ่งค่าที่ได้จะถูกนำไปใช้ในการคำนวณค่า สภาพต้านทานไฟฟ้า ตามสูตรของ Ziman จากผลการคำนวณทำให้ได้ข้อสรุปในกรณีที่ฉนวนเปลี่ยนไปเป็นโลหะด้วยการให้ความดันว่าเกิดจาก ตำแหน่งของยอดแรกของ $S(k)$ ที่เลื่อนจากจุดที่มีค่าน้อยกว่า $2k_F$ ไปสู่จุดที่มีค่ามากกว่า

ภาควิชา ฟิสิกส์	ลายมือชื่อนิสิต ....
สาขาวิชา ฟิสิกส์	ลายมือชื่ออาจารย์ที่ปรึกษา ....
ปีการศึกษา 2544	ลายมือชื่ออาจารย์ที่ปรึกษาร่วม ....

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KEYWORD : PAIRDISTRIBUTION FUNCTION/ STRUCTURE FACTOR/ PERCUS - YEVICK

RANGSUN KONJANATNIKORN : PAIR DISTRIBUTION FUNCTION IN LIQUID HYDROGEN. THESIS ADVISOR : ASSOC. PROF. WICHIT SRITRAKOOL Ph.D., 61PP. , ISBN 974-03-1529-1.

Pair distribution function of liquid metallic hydrogen is calculated under any condition of densities, pressures, and temperatures, by using the Percus – Yevick approximation to solve the Ornstein – Zernike equation in case of hard – sphere atomic potential. The solution is dependent on the sphere radius which can be found from the equation of state when densities, pressures, and temperatures are known. By the same method, we calculate the structure factor $S(k)$ and use it to calculate the electrical resistivity following Ziman's formula. From the result, we can conclude that the insulator - metal transformation due to pressure occurs when the position of the first peak of $S(k)$ shifts from the value smaller than to the value greater than $2k_F$.

Department	Physics	Student's signature ....
Field of study	Physics	Advisor's signature ....
Academic year 2001		Co-advisor's signature ....

Capture radius of magnetic particles in random cylindrical matrices in high gradient magnetic separation

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An effective medium treatment (EMT) was used to model the magnetic field around randomly distributed magnetic cylindrical fine wires and applied to calculate the capture radius of paramagnetic particles in a filter operating either in the longitudinal or transverse design mode. This article reports capture radius as a function of the ratio of magnetic velocity to fluid entrance velocity with a magnetic parameter which determines the strength of the magnetic short-range force, as a parameter. Finally, comparisons of the results based on the EMT approach, with those obtained by using the single-wire model, are given along with discussion on the criteria for validity of the simple single-wire model. © *1999 American Institute of Physics.* [S0021-8979(99)00302-3]

I. INTRODUCTION

The theory of magnetic filtration has long been investigated; however, most of the theories published are based on the simplest single collector model. Among those, the formerly developed theory by Watson[1] has been referred to by many authors. This theory explains the capture of the weakly magnetic particles carried by fluid of potential flow type, defined by Reynold's number $\mathrm{Re}=\rho V_0 a/\eta \gg 1$, where ρ, V_0, η, and a are the fluid density, entrance velocity, viscosity, and collector radius, respectively. The theoretical model used consists of an isolated fine ferromagnetic cylindrical wire in the background of a uniform applied magnetic field. Later, Watson[2] calculated the capture radius of paramagnetic particles in a filter consisting of fine ferromagnetic wires using the same approach as reported in the previous publication.[1] This article includes analysis of the relation between the capture radius and the external uniform magnetic field with a magnetic parameter K_s which measures the short-range force as a parameter.

Particle capture in the random matrix at low field intensity limit has been treated by Sheerer *et al.*[3] The capture radius of a single wire with arbitrary orientation with respect to the applied magnetic field direction was evaluated and used to determine the mean capture radius in describing an overall filter efficiency. In this research, the single-wire theory is generalized and the results of Watson[2] are extended by using the effective medium treatment (EMT) to predict the magnetic field around the filter matrices consisting of parallel wires distributed randomly. The same treatment was applied to a similar system of random sphere assemblage presented by Moyer *et al.*[4,5] and Natenapit.[6] The capture radius results of this study were reported and compared with those of Watson[2] based on the single-wire model. Finally, the criteria for validity of the single-wire model used to determine magnetic field around the filter matrices are discussed.

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II. THE MAGNETIC FIELD AND FORCES

To determine the magnetic field around parallel cylindrical wires of high permeability, which are randomly distributed in a formerly uniform external magnetic field applied perpendicular to the wires' axes, the effective medium treatment originally conceived by Hashin[7] to describe the effective conductivity of spherical particulate composites was employed. In this approach, the system of magnetic cylinders and surrounding fluid medium is considered to be composed of cylindrical cells, each containing one of the cylinders. The ratio of the cylinder to cell volume (a^2/b^2) is set equal to the packing fraction of cylinders in the medium (F). Adjacent to each cylinder (permeability μ_s) is the surrounding fluid medium (permeability μ_f). In this model, only a representative cell is considered while the neighbor cells are replaced by a homogeneous medium with effective permeability μ^* to be determined. Self consistency is achieved by requiring the magnetic induction averaged over the composite cylinder (cylindrical wire plus fluid shell) to be the volume average of the magnetic induction over the effective medium[7] [see Eq. (A13)]. Taking $\mathbf{H}_0$ along x axis and the wire cross section on the xy plane, the following equations were obtained (see Appendix for details):

$$\mathbf{H}=AH_0\left[\left(1+\frac{K_c}{r_a^2}\right)\cos\theta\hat{r}-\left(1-\frac{K_c}{r_a^2}\right)\sin\theta\hat{\theta}\right],\quad 1<r_a<\frac{b}{a} \tag{1a}$$

$$=\mathbf{H}_0,\quad \frac{b}{a}<r_a<\infty, \tag{1b}$$

where $A=1/(1-FK_c)$, $K_c=(\nu-1)/(\nu+1)$, $\nu=\mu_s/\mu_f$, and $r_a=r/a$.

Alternatively and equivalently, the effective permeability has been defined interms of the magnetic energy integral and determined by using variational theorems.[8] The consistent expression for the effective permeability μ^* has been obtained. From Eq. (1a), one can see that the magnetization

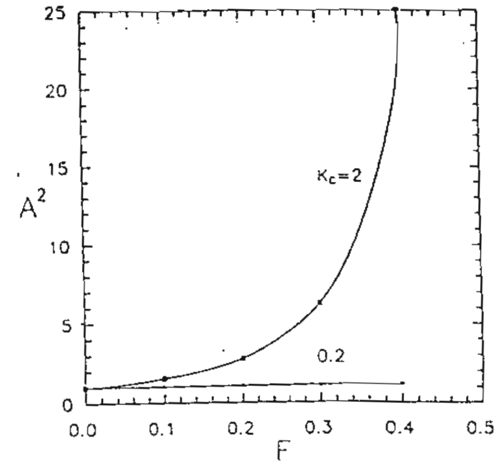

FIG. 1. A^2 as a function of packing fraction.

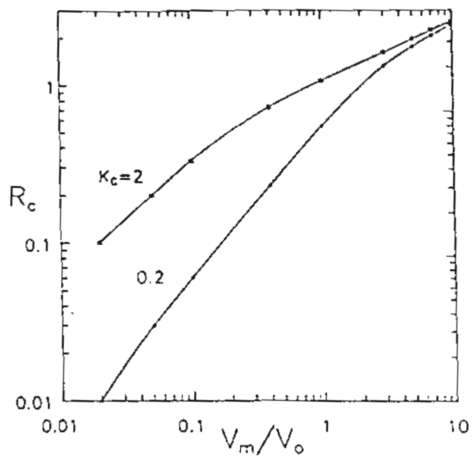

FIG. 2. Capture radius for paramagnetic particles as a function of V_m/V_0 for a longitudinal filter with packing fraction $F=0.0001$.

of the matrix increases the local field in the fluid shell, depending on the overall shape of the matrix volume and the magnetic parameter K_c. Equation (1b) is true for the EMT model used here, resulting from the boundary condition (i) in the Appendix and the obtained μ^* without further assumption on the magnetic field.

The magnetic force acting on a small particle of radius r_p and magnetic susceptibility χ_p located in the fluid of susceptibility χ_f is[9]

$$\mathbf{f}_m=\frac{2\pi}{3} r_p^3\mu_0\chi\nabla H^2, \quad \chi=\chi_p-\chi_f. \tag{2}$$

The particle is said to be paramagnetic if $\chi_p>\chi_f$ and diamagnetic if $\chi_p<\chi_f$.

Substituting H from Eq. (1) into Eq. (2), the magnetic force which depends on the particle radius, external field H_0, magnetic parameters K_c, and A^2 is obtained. Figure 1 shows the variation of A^2 as a function of the packing fraction for $K_c=0.2$ and 2. The other major force to be considered is the viscous drag force which is generally assumed to obey Stokes' law

$$\mathbf{f}_d=-6\pi\eta r_p(\mathbf{v}-\mathbf{v}_f). \tag{3}$$

Here, $\mathbf{v}_f$ is the fluid velocity, $\mathbf{v}=d\mathbf{r}/dt$ the particle velocity, and η the viscosity.

III. EQUATIONS OF MOTION

By using the magnetic field developed here and the single-wire potential flow field, the equations of motion similar to those reported by Watson[2] were obtained as follows:

$$\frac{dr_a}{dt}=\left(\frac{V_0}{a}\right)\left(1-\frac{1}{r_a^2}\right)\cos(\theta-\alpha)-\left(\frac{V_m}{a}\right)A^2\left(\frac{K_c}{r_a^5}+\frac{\cos 2\theta}{r_a^3}\right), \tag{4}$$

$$r_a\frac{d\theta}{dt}=-\left(\frac{V_0}{a}\right)\left(1+\frac{1}{r_a^2}\right)\sin(\theta-\alpha)-\left(\frac{V_m}{a}\right)A^2\frac{\sin 2\theta}{r_a^3}, \tag{5}$$

$$\frac{dz_a}{dt}=0, \tag{6}$$

where $\alpha=0$ or $\pi/2$ for a filter in longitudinal ($\mathbf{H}_0\|\mathbf{V}_0$) or transverse ($\mathbf{H}_0\perp\mathbf{V}_0$) design, respectively. Here, the magnetic velocity

$$V_m=\frac{4}{9}\frac{\chi\mu_0H_0^2r_p^2K_c}{\eta a}$$

is multiplied by the factor $A^2=1/(1-FK_c)^2$ to account for the influence of the neighboring wires on the pattern of magnetic field around the filter matrices. It is noted that the magnetic parameter K_c is equivalent to the familiar magnetic parameter $K_s=M_s/(2\mu_0H_0)$ for a single-wire model. For a normal matrix with a very low coercive force, the maximum value of $K_s=1$. $K_s>1$ can only occur for an hysteretic matrix.[10]

The equations of motion are solved numerically for particle trajectories at varying initial positions on the xy plane. The inspection of the particle trajectories yields the critical capture radius (R_c) which depends on the following parameters: V_m/V_0, F, and K_c.

IV. RESULTS AND DISCUSSION

In this research, capture radius for paramagnetic particles as a function of the ratio of magnetic velocity to fluid entrance velocity (V_m/V_0) in both longitudinal ($\mathbf{H}_0\|\mathbf{V}_0$) and transverse ($\mathbf{H}_0\perp\mathbf{V}_0$) magnetic filters with parameters $K_c=0.2$ and 2 were determined. Three cases of the magnetic filters with different values of packing fraction are considered. First, for a very dilute limit of filter packing fraction ($F=0.0001$), R_c as a function of V_m/V_0 is shown in Figs. 2 and 3. In this limit of packing fraction, $A^2\cong 1$ for all values of K_c as can be observed from Fig. 1. This indicates that the EMT results of R_c obtained are consistent with the corresponding single-wire model results reported by Watson.[2] These are confirmed for the case of magnetic filters operating in longitudinal and transverse modes as shown in Figs. 2 and 3, respectively. Furthermore, Fig. 1 also indicates that the single-wire model is a good approximation for all values of K_c up to filter packing fraction $F\sim 0.05$.

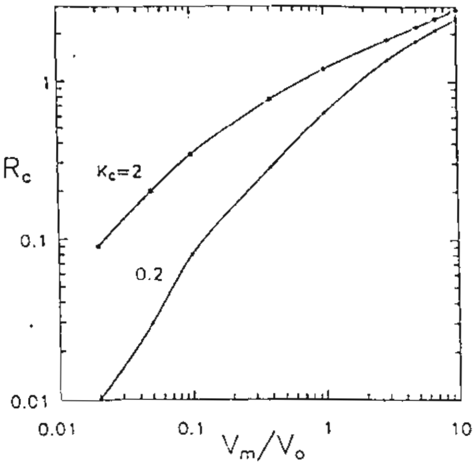

FIG. 3. Capture radius for paramagnetic particles as a function of V_m/V_0 for a transverse filter with packing fraction $F=0.0001$.

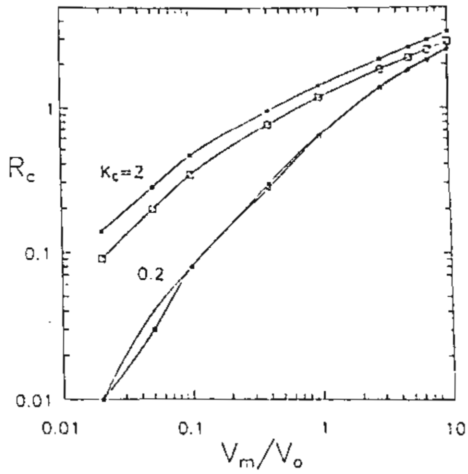

FIG. 5. Capture radius for paramagnetic particles as a function of V_m/V_0 based on EMT (*,*) and single-wire (□, ▢) magnetic fields for a transverse filter with packing fraction $F=0.1$.

Second, for a filter packing fraction $F=0.1$, the relation between R_c and V_m/V_0 based on the EMT magnetic field developed here, are compared with those based on the single-wire model as shown in Figs. 4 and 5 for longitudinal and transverse modes, respectively. Again two values of $K_c=0.2$ and 2 were used. For all cases, the EMT results for R_c are higher than the corresponding single-wire model results; however, the difference is insignificant for $K_c=0.2$, especially for the longitudinal mode. Thirdly, for a higher value of packing fraction ($F=0.2$), the similar dependence of R_c on V_m/V_0 are illustrated in Figs. 6 and 7 for the longitudinal and transverse modes, respectively. Here the difference between the EMT and single-wire results for $K_c=2$ is more pronounced than the former case of a lower packing fraction $F=0.1$. However, the difference is still very little for the smaller magnetic parameter $K_c=0.2$.

V. CONCLUSION

The two-dimensional description of the flow field around cylindrical matrix wires is applied to a three-dimensional problem and the geometry used is similar to that used by Kuwabara[11] to discuss the flow around cylindrical matrix wires. It should be noted that the changes in flow produced by the presence of the wire falls as r_a^{-2} and so these are considerably more important at low operating parameter V_m/V_0, than the changes in magnetic field produced by the matrix where there is a r_a^{-3} and a r_a^{-5} dependence for cylinders. In the case of spheres, the fall off is even more rapid[12] and the capture for a system of randomly packed spheres is dominated by the short-range term r_a^{-7}.

The studies also indicate that the effects of neigboring wires on the magnetic field pattern around the filter matrices may be neglected for a small packing fraction, e.g., F

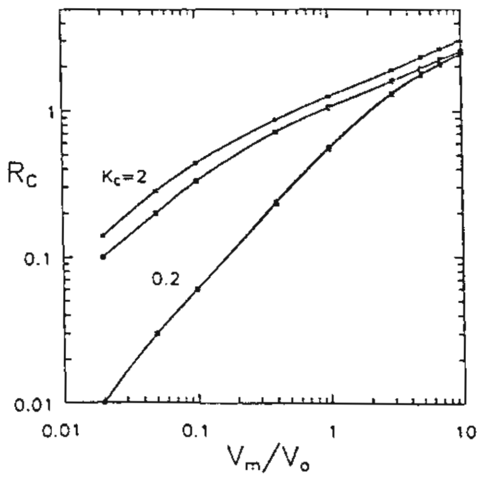

FIG. 4. Capture radius for paramagnetic particles as a function of V_m/V_0 based on EMT (*,*) and single-wire (□, ▢) magnetic fields for a longitudinal filter with packing fraction $F=0.1$.

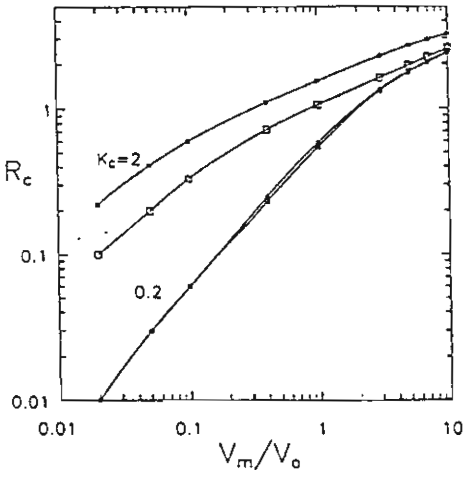

FIG. 6. Capture radius for paramagnetic particles as a function of V_m/V_0 based on EMT (*,*) and single-wire (□, ▢) magnetic fields for a longitudinal filter with packing fraction $F=0.2$.

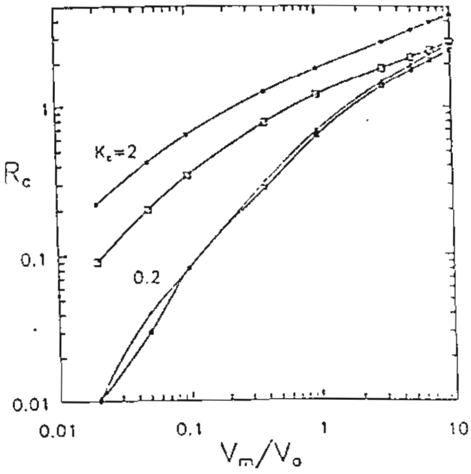

FIG. 7. Capture radius for paramagnetic particles as a function of V_m/V_0 based on EMT (•,*) and single-wire (□, ⌷) magnetic fields for a transverse filter with packing fraction $F=0.2$.

$\cong 0.05$, for all possible values of the magnetic parameter K_c which determines the strength of the magnetic short-range force [r_a^{-5} term in Eq. (4)]. Here K_c depends on the ratio of the wire permeability to fluid permeability as $K_c=(\mu_s/\mu_f-1)/(\mu_s/\mu_f+1)$. However, for a higher packing fraction, the single-wire approximation is still good only for the lower values of K_c (say <0.2).

ACKNOWLEDGMENTS

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APPENDIX

To determine the magnetic field in the cell, the boundary value problem of coaxial magnetic cylinders subject to the boundary condition of uniform magnetic field at far away from the cylindrical cell is solved. Taking z axis of cylindrical coordinate along the cylinder axis and let φ be the magnetic potential satisfying Laplace's equation for each region

$$\nabla^2\varphi_0=0, \quad b<r<\infty, \tag{A1}$$

$$\nabla^2\varphi_1=0, \quad a<r<b, \tag{A2}$$

$$\nabla^2\varphi_2=0, \quad 0<r<a \tag{A3}$$

with the boundary conditions

(i) $\varphi_0(r,\theta)=-H_0 r\cos\theta$ at $r\rightarrow\infty$,

(ii) $\dfrac{\partial\varphi_0(b,\theta)}{\partial\theta}=\dfrac{\partial\varphi_1(b,\theta)}{\partial\theta}$,

(iii) $\dfrac{\partial\varphi_1(a,\theta)}{\partial\theta}=\dfrac{\partial\varphi_2(a,\theta)}{\partial\theta}$,

(iv) $\mu^*\dfrac{\partial\varphi_0(r,\theta)}{\partial r}\bigg|_{r=b}=\mu_f\dfrac{\partial\varphi_1(r,\theta)}{\partial r}\bigg|_{r=b}$,

and

(v) $\mu_f\dfrac{\partial\varphi_1(r,\theta)}{\partial r}\bigg|_{r=a}=\mu_s\dfrac{\partial\varphi_2(r,\theta)}{\partial r}\bigg|_{r=a}$.

The general solutions of Laplace's Eqs. (A1)–(A3) are

$$\varphi_0(r,\theta)=-H_0 r\cos\theta+\sum_{n=1}^{\infty}A_n r^{-n}\cos n\theta, \tag{A4}$$

$$\varphi_1(r,\theta)=\sum_{n=1}^{\infty}[B_n r^n+C_n r^{-n}]\cos n\theta, \tag{A5}$$

and

$$\varphi_2(r,\theta)=\sum_{n=1}^{\infty}D_n r^n\cos n\theta, \tag{A6}$$

where the boundary condition (i) was imposed.

Applying the boundary conditions (ii)–(v), the constant coefficients were obtained as follows:

$$A_n=B_n=C_n=D_n=0, \quad \text{for } n\neq 1, \tag{A7}$$

$$A_1=\frac{H_0 a^2}{IF}[F(\nu^*+1)(\nu-1)-(\nu^*-1)(\nu+1)], \tag{A8}$$

$$B_1=-\frac{2H_0\nu^*}{I}(\nu+1), \tag{A9}$$

$$C_1=\frac{2H_0 a^2\nu^*}{I}(\nu-1), \tag{A10}$$

and

$$D_1=-\frac{4H_0\nu^*}{I}, \tag{A11}$$

where $\nu^*=\mu^*/\mu_f$, $\nu=\mu_s/\mu_f$, and $I=[(\nu^*+1)(\nu+1)-F(\nu-1)(\nu^*-1)]$.

The magnetic field related to φ by

$$\mathbf{H}=-\nabla\varphi \tag{A12}$$

is now obtained everywhere by inserting Eqs. (A4)–(A11) into the above equation. However, the results are given interms of the unknown effective permeability μ^*. μ^* is determined self consistency by requiring the magnetic induction averaged over the composite cell (cylinder plus cell medium) to be the volume average of the magnetic induction over the effective medium. That is,

$$F\mu_s\langle \mathbf{H}_2\rangle_i+(1-F)\mu_f\langle \mathbf{H}_1\rangle_i=\mu^*\langle \mathbf{H}_{\text{eff}}\rangle_i, \quad (\mathbf{H}_{\text{eff}}=-\nabla\varphi_0), \tag{A13}$$

where i referred to x, y, or z. Substituting the magnetic field into Eq. (A13) and taking the x component, we obtain the relative effective permeability

$$\nu^*=\frac{\nu(1+F)+(1-F)}{\nu(1-F)+(1+F)}, \quad \left(\nu^*=\frac{\mu^*}{\mu_f}, \nu=\frac{\mu_s}{\mu_f}\right). \tag{A14}$$

Then, the magnetic fields in the cell and the effective medium are obtained as

$$\mathbf{H}=AH_0\left[\left(1+\frac{K_c}{r_a^2}\right)\cos\theta\hat{r}-\left(1-\frac{K_c}{r_a^2}\right)\sin\theta\hat{\theta}\right],$$

$$1<r_a<\frac{b}{a} \tag{A15a}$$

$$=\mathbf{H}_0,\quad b/a<r_a<\infty, \tag{A15b}$$

where $A=1/(1-FK_c)$, $K_c=(\nu-1)/(\nu+1)$, and $r_a=r/a$.

We note that in the limit of $F(=a^2/b^2)\to 0$, $\nu^*=1$ (or $\mu^*=\mu_f$), and Eq. (A15a) is reduced to the single cylinder solution as expected. For $\mu_s=\mu_f$ (i.e. $K_c=0$, $A=1$), the homogeneous magnetic field $\mathbf{H}=\mathbf{H}_0$ is obtained.

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Electronic transport properties of Sierpinski lattices

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We have studied the electronic transport properties of open Sierpinski gasket systems connected to two electron reservoirs in the presence of a magnetic field. In the framework of a tight-binding model, the systems are composed of one-dimensional ordered chains. A generalized eigenfunction method, which allows one to deal with finite systems consisting of a large number of lattice sites (nodes), is used to calculate the transmission and reflection coefficients of the studied systems. The numerical results show that there are two kinds of symmetries of the transmission coefficient T to magnetic flux Φ, and there are antiresonant state regions ($T=0$) and resonant states ($T=1$). It is different from the open ring systems now the electronic energies of resonant states do not coincide with the eigenenergies of the isolated Sierpinski gasket systems. It is also found that the transmission behavior of the single exit systems is much more complicated than that of two exit systems. [S0163-1829(99)03640-1]

I. INTRODUCTION

In the past decade, rapid progress has been made in the area of mesoscopic physics. Quantum transport in mesoscopic systems has been extensively studied both experimentally and theoretically.[1–19] For mesoscopic systems at very low temperatures, the scattering due to phonons, which is a dephasing scattering, is significantly suppressed and the phase-coherence length of electrons becomes large compared to the system dimension. The scattering in the systems can then be modeled as phase-coherent elastic scatterings. Furthermore, if we consider the electron as a free particle, an idealized sample becomes an electron waveguide, which assumes that the electron transport through the system is perfectly ballistic. In recent years, there have been many works devoted to the study of the electronic properties of mesoscopic systems within the framework of the waveguide theory[9–14] and the tight-binding model.[7,8,15–19] Along these lines, the theoretical work to date has focused largely on the problems related to an isolated ring, or to open ring systems connected via leads to electronic reservoirs together with a magnetic flux Φ through the rings. For an isolated ring, the persistent current has been the focus of attention.[3–6] The idea is based on the possibility that the electron wave function may extend coherently over the whole circumference of the ring, and elastic scatterings, finite temperature, and weak inelastic scatterings do not destroy the coherence. As for the open ring systems, the important problem is to study the relationship among the transmission coefficient T, incident electron energy E, and magnetic flux Φ through the rings. The electron reservoirs in the open ring systems act as the source of energy dissipation or irreversibility, and all scattering processes in the leads and rings are assumed to be elastic. Based on the waveguide theory, Xia[10] has studied the Aharonov-Bohm effect in an open ring by calculating the transmission and reflection amplitudes as functions of the magnetic flux, the arm length, and the wave vector. Singha Deo and Jayannavar[12,13] have studied the quantum transport properties of serial stub or ring structures and the band formation in these geometries. Takai and Ohta[14] have published a series of articles investigating similar problems in the presence of both an electrostatic potential and magnetic flux.

On the other hand, it is well known that the tight-binding model is more flexible in theoretical treatments than the waveguide theory as disorder can be introduced readily and the band-structure effects are included.[20,21] Along these lines, Entin-Wohlman *et al.*[7] and Kowal *et al.*[8] have studied the electronic transport properties of an open single ring. Aldea *et al.*[11] studied the same problems using the Green's-function method. Wu and Mahler[9] have developed the quantum network theory of transport, by which the transmission probability for an open *A-B* type ring with an arbitrary form factor has been studied in detail. Liu and co-workers have investigated the persistent current of an isolated disordered ring,[15] the effects of spin interaction on the persistent current,[16] as well as the electronic transport properties of variant ring systems threaded by magnetic flux.[17–19]

Fractals and their properties have been studied by physicists for many years. Lakhtakia *et al.* have studied the construction and the analytic properties of the fractal clusters, and they also investigated the diffusion motion of the Pascal-Sierpinski gaskets by using combinational algebra.[20] For electronic transmission, the fractal lattices are much more complicated in structure compared with the ring systems. One of the main points of interest has been the fact that these self-similar objects are found to serve as a nontrivial model

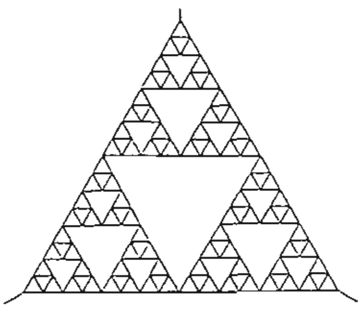

FIG. 1. The fourth-generation Sierpinski gasket lattice, the electronic properties of which are studied in the text.

for the backbone of transport problems. Fractals, in particular deterministic fractals such as the Sierpinski gasket (SG) fractal, possess some special properties, one of which is scale invariance, and do not have any translational order. They in fact bridge the gap between periodic and disordered systems.[22] Therefore, a detailed study on the electronic properties of fractals would lead to new physical results and increase our understanding of nonperiodic systems. Even though there is a large volume in the literature concerned with fractal systems, the study of their electronic properties is not that exhaustive. Along these lines, the energy spectrum and localization of electronic states in an isolated Sierpinski gasket lattice (SGL) have been the subject of many papers.[23–27] Domany *et al.*[23] studied the energy spectrum of the isolated SGL by the use of the recursive technique. Rammal and Toulouse[24] investigated the same problem in the presence of a magnetic field. However, in recent years the belief has been that in a highly correlated self-similar fractal system, such as SGL, localized eigenstates can exist. This should be a kind of structure-induced localization, which is different from Anderson localization due to incoherent scattering.[21] Therefore, the electronic transport properties of this kind of fractal structure would be an interesting problem. Chakrabarti[26] has found that in the absence of magnetic field for the isolated SGL, there are extended electron states. Wang[27] has studied the electronic localization of Sierpinski lattices, and claimed that there exist an infinite number of extended states. He has also studied the magnetic-field effects on the electronic states of the isolated SGL. But to the best of our knowledge, up to now the study on the electronic transport properties of an open SGL has not been reported yet. The reason would be that to deal with an electronic transmission problem of an open SGL, one would have to solve a united equation set, in which the number of equations roughly equals the number of the sites included in the SGL. Therefore, even for a finite SGL, this is a difficult work. Fortunately, we have found an effective approach to solve this problem, in which the transmission and reflection amplitudes are treated together with the electronic wave functions in the sites of the SGL, so that we can deduce a simpler formula to calculate the transmission and reflection coefficients. We have named this approach the generalized eigenfunction method (GEM). By the use of this GEM we have investigated the electronic transport properties of open SGL up to its fourth-generation system containing 123 sites (nodes), which is shown in Fig. 1. By the way, this GEM is formally similar to the fast multipole method (FMM), which is commonly used in electromagnetic scattering problems, but we should point out that they are essentially different from each other.[28] The main purpose of this paper is to investigate the behavior of the transmission coefficient T as the incident electron energy E and the magnetic flux Φ, which penetrates the elementary triangles of the SGL, are varied. Detailed results are given in three-dimensional plots of T against E and Φ, and of which in the two-dimensional cross sections T versus E. It is found that there are two kinds of symmetries of transmission coefficient T to flux Φ. The transmission behavior of single-exit SGL systems is much more complicated than that of two-exit systems. We also found that as the SGL generation increases, the antiresonant regions corresponding to $T=0$ in the E-Φ space progressively increase in both the region number and the region area. This means that in these regions the magnetic flux completely blocks out the electronic transport. This is an interesting quantum phenomenon. On the other hand, we have also calculated the eigenenergy spectrum of the corresponding isolated SGL, and found that in the open SGL case the electron energies of resonant transmission states do not coincide with the eigenenergies of the isolated SGL, which is different from the open ring systems.[18]

This paper is organized as follows. In Sec. II, we introduce the generalized eigenfunction method (GEM) to calculate the transmission and reflection coefficients of an open SGL. The numerical results and discussion of the electronic transport properties are presented in Sec. III. A brief summary is given in Sec. IV.

II. GENERALIZED EIGENFUNCTION METHOD AND ITS APPLICATION IN OPEN SGL SYSTEMS

For the studied open Sierpinski gasket lattices (SGL) which are coupled to two reservoirs via ideal leads, we assume that the leads connected to neighboring sites are composed of one-dimensional ordered chains with on-site energy ε_n and transfer integral t between nearest-neighboring sites. Denoting the incident electron energy by E and the projection of the Wannier wave function on the nth site by ψ_n, in the presence of a magnetic flux Φ the tight-binding equation can be written as[19]

$$(\varepsilon_n - E)\psi_n = \sum_{n'} t_{n,n'}\psi_{n+n'}, \tag{1}$$

where the transfer integral $t_{n,n'}$ equals $te^{\pm i2\pi\Phi/(\Phi_0 S)}$, the $S=3$ is the circumference length of the elementary triangle of the SGL, the magnetic phase $\phi = 2\pi\Phi/(\Phi_0 S)$, the $\Phi_0 = hc/e$ is the elementary flux quantum, and the sum runs over the nearest neighbors of site n. The wave function ψ_n can be written as the linear combination[18]

$$\psi_n = Ae^{ikn} + Be^{-ikn}, \tag{2}$$

where k is the wave vector, n is the site number, and we take the lattice distance to be unity. In the tight-binding model, the wave vector k is related with the incident electronic en-

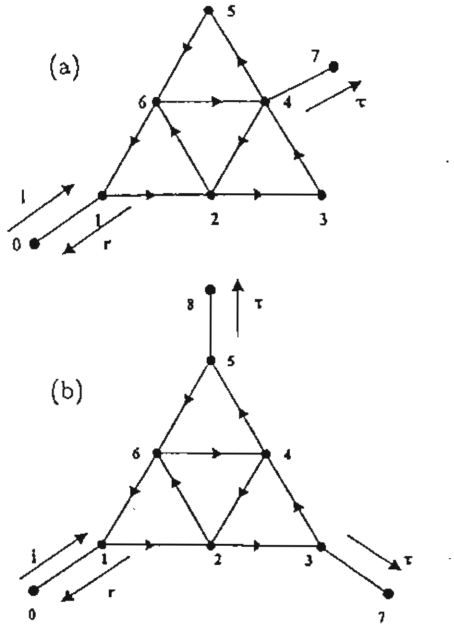

FIG. 2. First-generation Sierpinski lattice coupled to two reservoirs via ideal leads. The magnetic phase is equal to ϕ in the direction of the arrow and $-\phi$ otherwise. (a) One-exit case. (b) Two-exit case; both exits are coupled to the same reservoirs via ideal leads.

ergy E by formula $E=2t\cos k$. We first consider the first-generation SGL with a single exit shown in Fig. 2(a). By the use of Eq. (1) we obtain the tight-binding equations on the sites of the SGL as follows:

$$
\begin{aligned}
E\psi_1&=te^{-i\phi}\psi_2+te^{-i\phi}\psi_6+t\psi_0,\\
E\psi_2&=te^{i\phi}\psi_1+te^{-i\phi}\psi_3+te^{i\phi}\psi_4+te^{-i\phi}\psi_6,\\
E\psi_3&=te^{i\phi}\psi_2+te^{-i\phi}\psi_4,\\
E\psi_4&=te^{-i\phi}\psi_2+te^{i\phi}\psi_3+te^{-i\phi}\psi_5+te^{i\phi}\psi_6+t\psi_7,\\
E\psi_5&=te^{i\phi}\psi_4+te^{-i\phi}\psi_6,\\
E\psi_6&=te^{-i\phi}\psi_1+te^{i\phi}\psi_2+te^{-i\phi}\psi_4+te^{i\phi}\psi_5.
\end{aligned}
\tag{3}
$$

On the other hand, for the special sites located in the entry and exit we can write their wave function as[19]

$$
\begin{aligned}
\psi_0&=1+r \quad (n=0),\\
\psi_1&=e^{ik}+re^{-ik} \quad (n=1),\\
\psi_4&=\tau \quad (n=0),\\
\psi_7&=\tau e^{ik} \quad (n=1),
\end{aligned}
\tag{4}
$$

where r and τ are the reflection and transmission amplitudes of reflecting and outgoing wave functions, respectively. To calculate both of them, we have to solve the above united equation set (3) and (4); evidently this is difficult. If we consider higher-generation SGL, then obtaining an analytic solution seems impossible. To numerically solve this problem, we introduce the following generalized eigenfunction method (GEM). The trick of the GEM is that we treat the amplitudes r and τ the same as the wave functions ψ_i. In this way the united equation set (3) and (4) can be rewritten as the following $(N+2)$-order matrix equation. N is the number of sites in the SGL:

$$
\begin{bmatrix}
E & e^{-i\phi} & 0 & 0 & 0 & e^{i\phi} & 1 & 0\\
e^{i\phi} & E & e^{-i\phi} & e^{i\phi} & 0 & e^{-i\phi} & 0 & 0\\
0 & e^{i\phi} & E & e^{-i\phi} & 0 & 0 & 0 & 0\\
0 & e^{-i\phi} & e^{i\phi} & E & e^{-i\phi} & e^{i\phi} & 0 & e^{ik}\\
0 & 0 & 0 & e^{i\phi} & E & e^{-i\phi} & 0 & 0\\
e^{-i\phi} & e^{i\phi} & 0 & e^{-i\phi} & e^{i\phi} & E & 0 & 0\\
1 & 0 & 0 & 0 & 0 & 0 & -e^{-ik} & 0\\
0 & 0 & 0 & 1 & 0 & 0 & 0 & -1
\end{bmatrix}
\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\\ \psi_4\\ \psi_5\\ \psi_6\\ r\\ \tau\end{pmatrix}
=
\begin{pmatrix}-1\\ 0\\ 0\\ 0\\ 0\\ 0\\ e^{ik}\\ 0\end{pmatrix}.
\tag{5}
$$

For the sake of simplicity, in the above equation we have chosen $\varepsilon_n=0$ and $t=1$.

If we denote the above matrix equation (5) as

$$M\Psi=C,$$

then the reflection and transmission amplitudes are simply

$$r=(M^{-1}C)_{N+1}, \quad \tau=(M^{-1}C)_{N+2}, \tag{6}$$

and the transmission coefficient $T=|\tau|^2$.

Here we would like to emphasize two points. First, the numerical solution of the above formula (6) is very easy to obtain even with a personal computer. Second, the above generalized eigenfunction method is a very powerful approach to deal with the electronic transport problems in lattice (network) systems, no matter how many entries and exits exist in the studied systems. Even for the quasiperiodic and disordered ones, and for three-dimensional systems, this GEM can also be very efficiently used. For example, the matrix equation of the first-generation SGL with *two exits* shown in Fig. 2(b) can be easily written as follows:

$$\begin{bmatrix} E & e^{-i\phi} & 0 & 0 & 0 & e^{i\phi} & 1 & 0 & 0 \\ e^{i\phi} & E & e^{-i\phi} & e^{i\phi} & 0 & e^{-i\phi} & 0 & 0 & 0 \\ 0 & e^{i\phi} & E & e^{-i\phi} & 0 & 0 & 0 & e^{ik} & 0 \\ 0 & e^{-i\phi} & e^{i\phi} & E & e^{-i\phi} & e^{i\phi} & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{i\phi} & E & -i\phi & 0 & 0 & e^{ik} \\ e^{-i\phi} & e^{i\phi} & 0 & e^{-i\phi} & e^{i\phi} & E & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & -e^{-ik} & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -1 \end{bmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \\ \psi_5 \\ \psi_6 \\ r \\ \tau_1 \\ \tau_2 \end{pmatrix} = \begin{pmatrix} -1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ e^{ik} \\ 0 \\ 0 \end{pmatrix}, \tag{7}$$

which is now an $(N+3)$-order matrix equation. In deducing the above matrix equation (7) we have used the following relations held in sites 3 and 5 of Fig. 2(b):

$$E\psi_3 = te^{i\phi}\psi_2 + te^{-i\phi}\psi_7 + t\tau_1 e^{ik},$$

$$E\psi_5 = te^{i\phi}\psi_4 + te^{-i\phi}\psi_6 + t\tau_2 e^{ik}.$$

The corresponding reflection and transmission amplitudes of reflecting and outgoing wave functions are, respectively,

$$r = (M^{-1}C)_{N+1}, \quad \tau_1 = (M^{-1}C)_{N+2}, \quad \tau_2 = (M^{-1}C)_{N+3}. \tag{8}$$

From the above example we can see that in the same way we can easily extend the GEM to multientries (and exits) cases. To clarify the name GEM, we should compare the generalized eigenfunction equation (5) with the energy eigenvalue matrix equation of an *isolated* SGL written in the following. If we assume the site energy $\epsilon_n = 0$ for the whole system, then the tight-binding equations in the sites and their corresponding eigenvalue matrix equation are, respectively,

$$\begin{aligned} E\psi_1 &= te^{-i\phi}\psi_2 + te^{-i\phi}\psi_6, \\ E\psi_2 &= te^{i\phi}\psi_1 + te^{-i\phi}\psi_3 + te^{i\phi}\psi_4 + te^{-i\phi}\psi_6, \\ E\psi_3 &= te^{i\phi}\psi_2 + te^{-i\phi}\psi_4, \\ E\psi_4 &= te^{-i\phi}\psi_2 + te^{i\phi}\psi_3 + te^{-i\phi}\psi_5 + te^{i\phi}\psi_6, \\ E\psi_5 &= te^{i\phi}\psi_4 + te^{-i\phi}\psi_6, \\ E\psi_6 &= te^{-i\phi}\psi_1 + te^{i\phi}\psi_2 + te^{-i\phi}\psi_4 + te^{i\phi}\psi_5, \end{aligned} \tag{9}$$

and

$$\begin{bmatrix} E & e^{-i\phi} & 0 & 0 & 0 & e^{i\phi} \\ e^{i\phi} & E & e^{-i\phi} & e^{i\phi} & 0 & -i\phi \\ 0 & e^{i\phi} & E & e^{-i\phi} & 0 & 0 \\ 0 & e^{-i\phi} & e^{i\phi} & E & e^{-i\phi} & e^{i\phi} \\ 0 & 0 & 0 & e^{i\phi} & E & e^{-i\phi} \\ e^{-i\phi} & e^{i\phi} & 0 & e^{-i\phi} & e^{i\phi} & E \end{bmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \\ \psi_5 \\ \psi_6 \end{pmatrix} = 0, \tag{10}$$

where we can see that the above N-order square matrix is the submatrix of matrix $\mathbf{M}$ of the matrix equation (5), and the above eigenwave function vector is the subvector of the corresponding vector of matrix equation (5). That is why we call the method the generalized eigenfunction method.

III. NUMERICAL RESULTS AND DISCUSSION

The formalism mentioned in Sec. II can be easily implemented numerically and the results for both the single- and two-exit cases are obtained up to fourth-generation open SGL with site (node) number $N=123$. The numerical calculation is easy and quick even with a personal computer. Because the main characters of the transport properties have been revealed in the investigation of the first four generation SGL, it is not necessary to consider the higher-generation systems. In our calculations, the on-site energies are chosen to be $\epsilon_n = 0$ and the transfer integrals $t=-1.0$. To examine the accuracy of our numerical calculations, we check at every intermediate stage of the calculation that the criterion $|\tau|^2 + |r|^2 = 1$ for the transmission and reflection coefficients is satisfied to a tolerance of 10^{-14}. This accuracy enables us to examine with confidence the electronic transport properties of the open SGL.

We consider two basic cases of the open SGL with one and two exits, of which the first-generation systems are

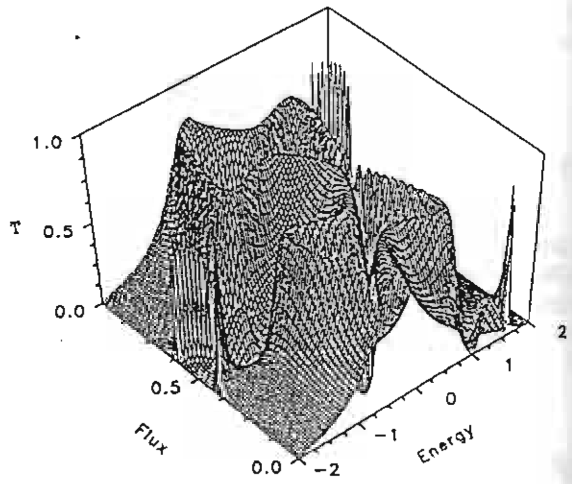

FIG. 3. Transmission coefficient T as a function of magnetic flux Φ and incident electron energy E for the first-generation Sierpinski lattice with a single exit.

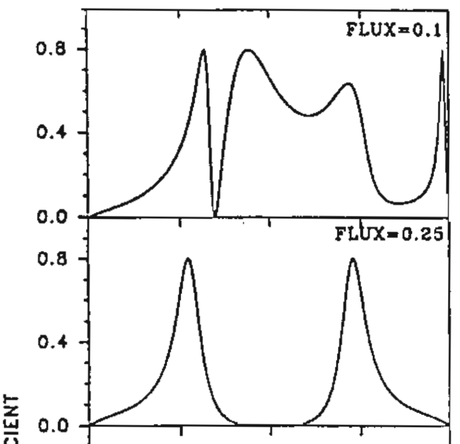

FIG. 4. Transmission coefficient T vs electron energy E as cross sections of Fig. 3. The corresponding flux is marked in the pictures. The two pictures are the same for $\Phi/\Phi_0=0.4$ and 0.6, but for $\Phi/\Phi_0=0.1$ and 0.4 they are "antisymmetric" to energy E (see text).

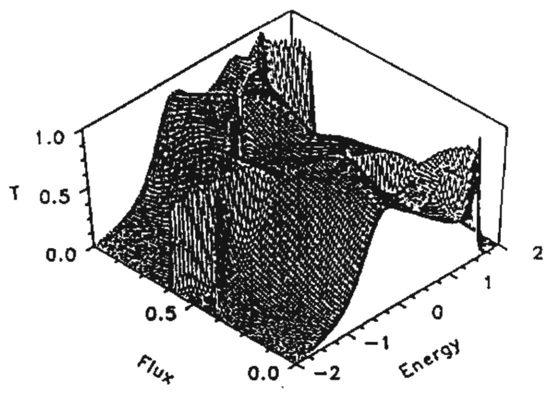

FIG. 5. Transmission coefficient T as a function of magnetic flux Φ and incident electron energy E for first-generation Sierpinski lattice with two exits.

shown in Fig. 2. By the use of the GEM, we have totally calculated the first four generation SGL. The numerical results are shown in Figs. 3–11, in which the typical three-dimensional plots of the transmission coefficient T against the electron energy E and magnetic flux Φ are shown in Figs. 3 and 5 for the first-generation SGL, in Figs. 7 and 8 for the second-generation SGL, in Fig. 10 for the third-generation SGL, and in Fig. 11 for the fourth-generation SGL. For the sake of clear visualization and because of the symmetry of the transmission spectrum, we plotted only a half and a quarter of the whole periodic picture in Figs. 10 and 11, respectively. To display the detail, we have also plotted some pictures of the transmission coefficient T versus energy E, i.e., the cross sections of three-dimensional plots, for the first-generation SGL in Fig. 4 (single exit) and Fig. 6 (two exits), and for the second-generation SGL with two exits in Fig. 9.

From the obtained numerical results, we can see some interesting transport properties, which exist in all studied SGL cases. First, following the enlargement of the SGL, the transmission coefficient T fluctuates more and more, i.e., there exist more and more peaks, valleys, and more and bigger zero-transmission ($T=0$) regions. This complexity of the transmission behaviors can be understood as the result of the quantum coherence effect among electrons traveling through the SGL. This is due to the fact that the presence of a magnetic flux destroys the time-reversal symmetry and the paths going clockwise and anticlockwise over the systems have different phases. Therefore, when the site number of the systems increases, the variant possibility of quantum coherence also increases, and the transmission coefficient as a function of the electron energy E and magnetic flux Φ becomes increasingly complicated. For the same reason, from the figures we can also see that the antiresonant state region, i.e., the region with $T=0$, enlarges following the increase of the site number. In Figs. 3 and 5 of the first-generation SGL there is no such region, but one does appear in Figs. 7 and 8 of the second-generation SGL and enlarges in the next generations. In the fourth generation SGL several such regions have appeared and their areas have quickly enlarged (see Fig. 11). This global behavior is clearly displayed in the three-dimensional T-E-Φ plots. To show the sophisticated relationship between the incident electron energy and its transmission coefficient, we have plotted the E versus T curves with $\Phi/\Phi_0=0.1$, 0.25, 0.4, 0.5, and 0.6, respectively, for the first- and second-generation SGL, and shown them in Figs. 4, 6, and 9, which compliment very well their corresponding 3D plots.

Second, we have noticed the symmetry of transmission behaviors. Because we need to use the eigenvalue matrix equation (10) to discuss the parameter symmetry of the transport property, we investigate in advance the relationship between the resonant electronic states of the *open* SGL and the energy eigenvalues of the *isolated* SGL. An incident electronic state with peak-value transmission coefficient T is called a resonant state. In the open ring systems the electronic energies of resonant states are close to the eigenenergies of the corresponding isolated ring systems.[18] An inter-

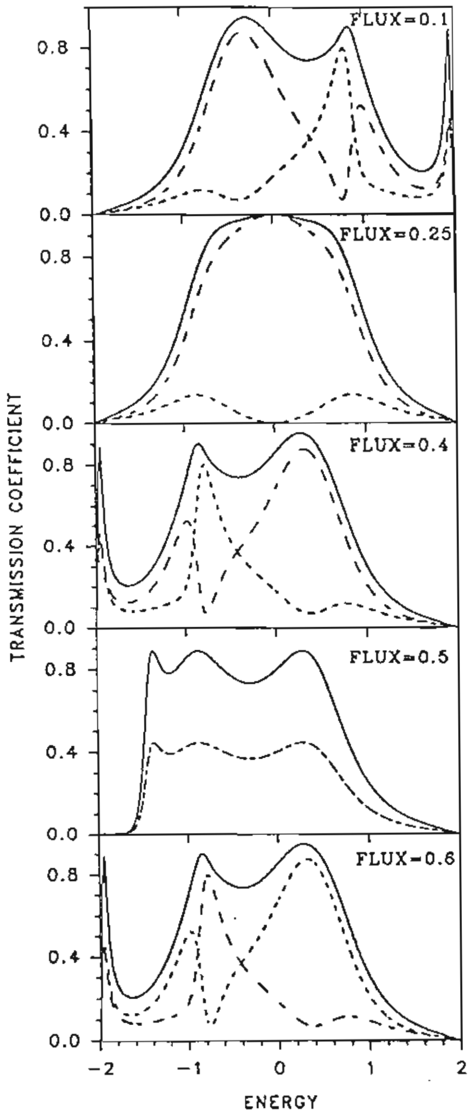

FIG. 6. Transmission coefficient T vs electron energy E as cross sections of Fig. 5. The corresponding flux is marked in the pictures. Long- and short-dashed lines are the transmission coefficients of exits 7 and 8, respectively. Solid lines are the sum of them. The plots show the same symmetry as the single-exit case (see text).

esting question is whether or not there exists the same kind of relationship in the SGL systems. Figure 12 shows the energy eigenvalue spectra of the isolated Sierpinski lattice for the first, second, and fourth generations, which are obtained by calculating Eq. (10). Comparing Fig. 12 with Figs. 3, 5, 7, 8, and 11, which show the T-Φ-E behaviors, we can see that in both the single- and two-exit cases, there is no definite correspondence between the electron energy of the resonant states of the open SGL and the eigenenergy of the isolated SGL. This means that the transport properties of the fractal systems are more complicated than those of the slab systems[13–14] and ring systems.[18] A plausible explanation for this phenomenon should be that the structure of the fractal systems is much more complicated than that of the ring systems, which leads to many more possibilities of variant reflection and transmission, so that quantum coherence effects have a much greater chance to influence the transport properties and finally destroy the correspondence of the two kinds of energies that exist in the open ring systems.

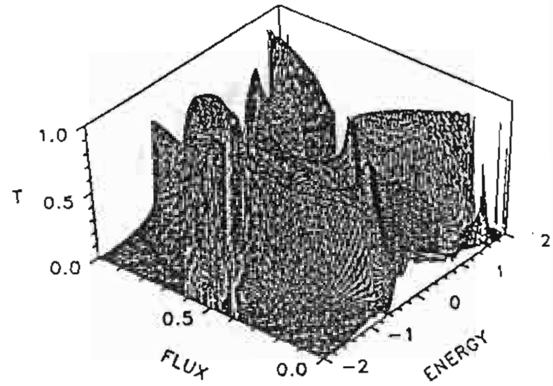

FIG. 7. Transmission coefficient T as a function of magnetic flux Φ and incident electron energy E for second-generation Sierpinski lattice with single exit.

On the other hand, from the energy spectra shown in Fig. 12 we have noticed that there are two kinds of symmetries. First, the energy spectrum is symmetric to $\Phi/\Phi_0=0.5$, i.e., for fluxes Φ/Φ_0 and $1-\Phi/\Phi_0$ two energy bands are exactly the same. Second, to the $\Phi/\Phi_0=0.25$ (or 0.75) the energy spectrum is "antisymmetric," i.e., there is a correspondence between $E(\Phi/\Phi_0)$ and $-E(0.5-\Phi/\Phi_0)$ for $\Phi/\Phi_0\leqslant 0.25$. This symmetrization of the energy spectrum could be understood from the eigenequation (10) of the first-generation SGL. We have obtained the polynomial expression satisfied by eigenenergies E:

$$-2-\cos 6\phi+6E\cos 3\phi-56E^3\cos 3\phi-480E^4+512E^6$$
$$=0, \tag{11}$$

from which we can see that the symmetry of the eigenenergy spectrum depends on the symmetry of $\cos 3\phi$, where

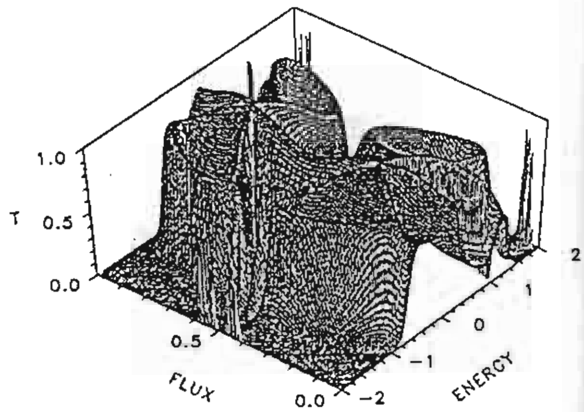

FIG. 8. Transmission coefficient T as a function of magnetic flux Φ and incident electron energy E for second-generation Sierpinski lattice with two exits.

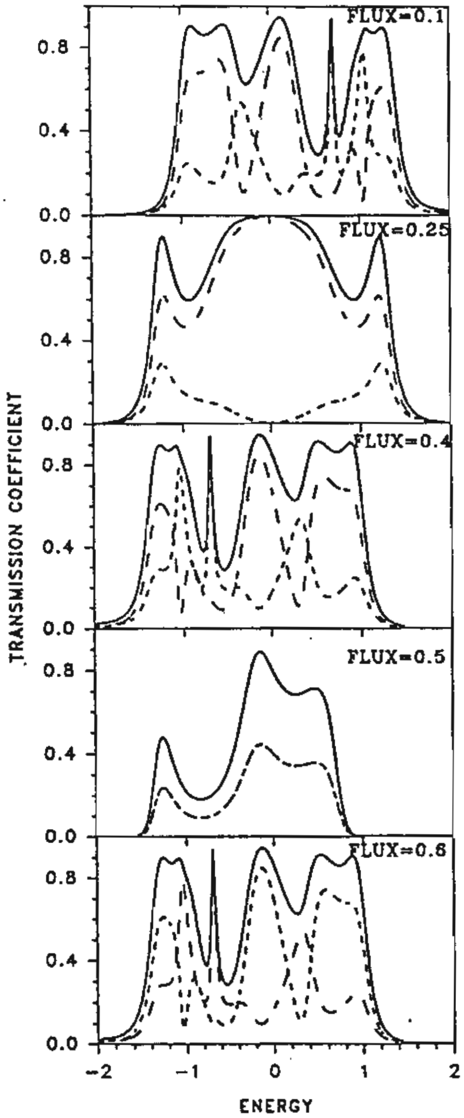

FIG. 9. Transmission coefficient T vs electron energy E as cross sections of Fig. 8. The corresponding flux is marked in the pictures. Long- and short-dashed lines are the transmission coefficients of exits 7 and 8, respectively. Solid lines are the sum of them. The plots show the same symmetry as the first-generation case (see text).

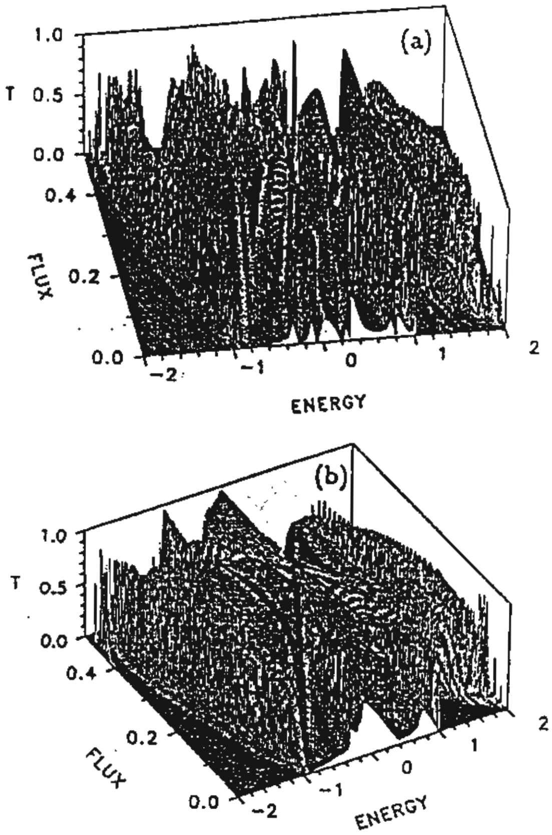

FIG. 10. Transmission coefficient T as a function of magnetic flux Φ and incident electron energy E for third-generation Sierpinski lattice. For the sake of clear visualization only a half-period in flux Φ is shown. (a) Single-exit case. (b) Two-exit case.

$\phi=2\pi\Phi/3\Phi_0$ so that $\cos 3\phi=\cos 2\pi\Phi/\Phi_0$. This is why there are $\Phi/\Phi_0=0.5$ and $\Phi/\Phi_0=0.25$ (0.75) kinds of symmetries, because they are merely the symmetries of $\cos 3\phi$. Here we can also see that the energy spectrum is periodic in flux with period $\Phi/\Phi_0=1$.

For the same reason, the transmission coefficient T also posseses these two kinds of symmetries. In the three-dimensional plots Figs. 3, 5, 7, and 8, we can find that there is a symmetric plane ($\Phi/\Phi_0=0.5,E$) and two symmetric centers ($\Phi/\Phi_0=0.25,E=0$) and ($\Phi/\Phi_0=0.75,E=0$). The symmetric centers are most clearly displayed in Fig. 8, which is a three-dimensional plot for the second-generation SGL with two exits. If we compare the generalized eigenequation (5) with the eigenenergy equation (10), we can see that in the matrix M of Eq. (5) the matrix elements related with flux Φ are exactly the same as those of the eigenenergy equation (10). Therefore, they have the same dependence on the flux Φ. For a better view, in Figs. 4 and 6 we show some T-E cross sections of the three-dimensional T-Φ-E plots, which show that the pictures of $\Phi/\Phi_0=0.4$ and 0.6 are exactly the same, and those of $\Phi/\Phi_0=0.4$ and 0.1 are "antisymmetric," i.e., $T(\Phi/\Phi_0,E)=T(0.5-\Phi/\Phi_0,-E)$. Therefore, the transmission coefficient T is symmetric for $\pm E$ in the $\Phi/\Phi_0=0.25$ case. This point is clearly shown in the two-dimensional plots Figs. 4 and 6. These similarities also originate from the same relationship to flux Φ for both of the matrix equations (5) and (10).

Another interesting phenomenon displayed in the figures is that the single-exit SGL shows more complicated transmission behavior than the two-exit systems, i.e., in the former the transmission spectrum contains more peaks, valleys, and bigger fluctuation. An intuitive explanation for this phenomenon could be that from Fig. 2(b) we can see that the two exits in the open SGL are symmetric, both of which directly connect with the entry site by a straight lead, which serves as a direct "transport channel." This means that for the two-exit systems the multiscattering effect and the quantum-coherent effect of structure are weaker compared with the single-exit systems.

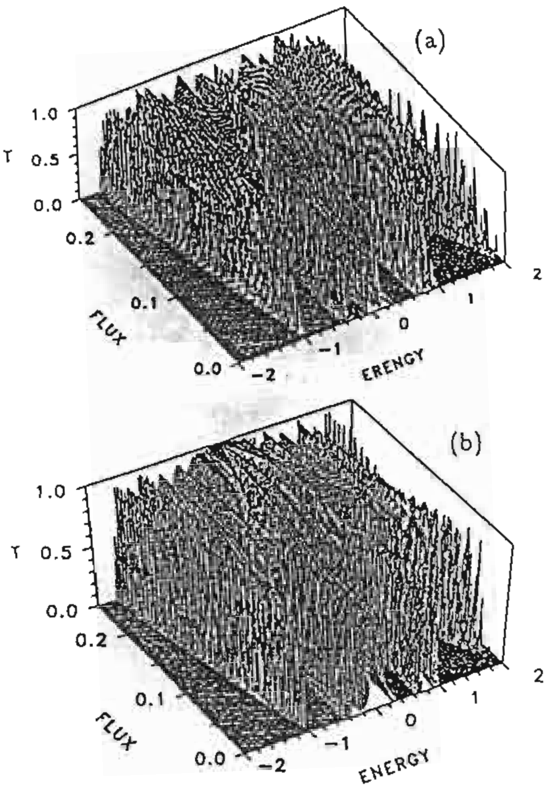

FIG. 11. Transmission coefficient T as a function of magnetic flux Φ and incident electron energy E for fourth-generation Sierpinski lattice. For the sake of clear visualization only a quarter of a period in flux Φ is shown. (a) Single-exit case. (b) Two-exit case.

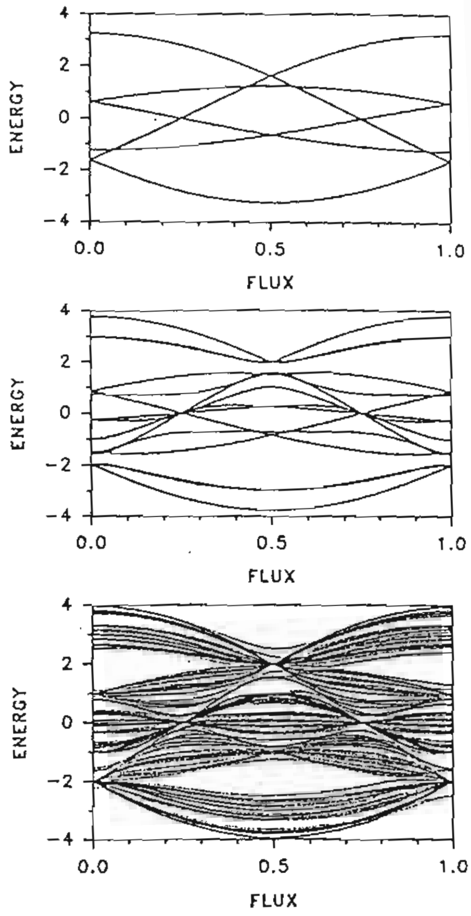

FIG. 12. Energy spectrum of isolated Sierpinski lattice as a function of magnetic flux Φ. From upper to bottom, they correspond to the first-, second-, and fourth-generation Shierpinski lattices, respectively. Readers should notice the symmetries of the spectrum to $\Phi/\Phi_0 = 0.5$ and 0.25.

In Figs. 6 and 9 we show the total and individual transmission coefficients T, T_1, T_2 for the first- and second-generation SGL with two exits. We can see the variation of the transmission coefficients T_1 and T_2 with the change of the magnetic flux Φ. Due to the modulation of the magnetic field, the T_1 and T_2 behaviors are different except in some special cases, such as $\Phi/\Phi_0 = 0$ and 0.5. Generally they periodically exchange the "position" following the variance of the flux Φ. This behavior comes from the fact that the two exits are symmetric in the structure of the SGL, therefore in the modulation of the magnetic field the T_1 and T_2 have a phase difference.

IV. BRIEF SUMMARY

We have introduced the generalized eigenfunction method (GEM), which is a very efficient and powerful approach to studying the electronic transport problems of aperiodic systems. By the use of the GEM we have studied the transport properties of open Sierpinski gasket lattices (SGL) coupled to two electron reservoirs via ideal leads. We have investigated the electronic transport properties of an open SGL up to its fourth-generation systems containing site number $N = 123$. The main purpose of this paper is to investigate the behavior of the transmission coefficient T as the incident electron energy E and the magnetic flux Φ, which penetrates the elementary triangles of the SGL, are varied. The detailed numerical results are given in three-dimensional plots of transmission coefficient T against electron energy E and flux Φ, and in which the two-dimensional cross sections are T versus E. It is found that following the enlargement of the SGL, the transmission coefficient T fluctuates more and more, there are more and more resonant peaks, low-transmission valleys, and more and bigger antiresonant states ($T = 0$) regions. In the transmission behaviors there are two kinds of symmetries to flux Φ. In the three-dimensional T-E-Φ plots, the transmission coefficient T has a symmetric plane ($\Phi/\Phi_0 = 0.5, E$) and two symmetric centers: ($\Phi/\Phi_0 = 0.25, E = 0$) and ($\Phi/\Phi_0 = 0.75, E = 0$). The numerical results show also that the transmission behavior of single-exit SGL systems is much more complicated than that of the two exit systems, because in the former there are direct "transport channels." It is different from the open ring systems now the electronic energies of the resonant states do not coincide with the eigenenergies of the isolated Sierpinski gasket systems. It means that the transport properties of the fractal systems are more complicated than those of the slab systems[13,14] and ring systems.[18] The above results increase our understanding of the transport properties of fractal systems. In the present paper, as an example, we only discussed the SG, which is a simple fractal gasket derived from the Pascal triangle modulo 2, but it is well known that other strictly self-similar gaskets can be derived from Pascal triangle modulo n when n is prime, and even for a nonprime n there also exists self-similarity in the asymptotic sense.[29,30] For these fractal structures, determining what kind of universal property there is in the electronic transport problem would be a very interesting problem, and worth studying.

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On the Specific Heat of the Cubic Quasicrystals

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ABSTRACT Based on the linear elasticity theory of the cubic quasicrystals, we have derived the equations of wave propagating in the cubic quasicrystals and the analytical expression of the phase velocity of wave propagation. Moreover, we extend the Debye hypothesis of continuous elastic medium to study the specific heat of the cubic quasicrystals, for which we obtain an analytic expression of the specific heat as well as an approach to calculate the Debye temperature Θ_D.

KEYWORDS: specific heat, elasticity wave, quasicrystal.

INTRODUCTION

Since the discovery of the icosahedral quasicrystal in Al-Mn alloys, the quasicrystals with noncrystallographic symmetry, such as decagonal, dodecagonal and octagonal phases have been extensively studied.[1-4] For resent years in the process of the rapid solidified $V_6Ni_{16}Si_7$ alloy, Feng *et al*[5-6] discovered a kind of quasicrystal with cubic symmetry, which has been a new subject in the field of quasicrystals. Wang *et al*[7] have discussed the projection description of the cubic quasicrystals and Yang *et al*[8] have studied their linear elasticity theory. There are still many physical properties of the cubic quasicrystals have not been studied yet. For example, one of the important physical properties, the specific heat of cubic quasicrystals has not been studied. It is well-known that for the general quasicrystals it is impossible to obtain an analytical solution of lattice vibration properties. Therefore it is impossible to get an analytic result for the physical properties related to the quasicrystal-lattice dynamics. Due to the special structure of the cubic quasicrystals, we can obtain some analytical results on its lattice dynamics. In the present article we will report our study on the specific heat of cubic quasicrystals. We have first derived the equation of wave propagation in the cubic quasicrystals and then obtained the specific heat expression of the cubic quasicrystals. It is well-known that the calculation of the specific heat for both of the crystals and quasicrystals has to base on the knowledge of their lattice vibration modes. In order to simplify the calculation, Debye[9] assumed that the lattice wave of the solid is an elastic wave of continuous medium. Based on this hypothesis he successfully obtained the specific heat formulas and explained the experimental phenomenon that the specific heat of crystals decrease by T^3 at low temperature. In this paper, following the Debye hypothesis we will extend the continuous medium model to the cubic quasicrystals, in which the contributions of the phonons, phasons and their couplings on the specific heat are considered in the six-dimensional space but the wave propagaation still exists in the physical spaee.[5-8] By this generalized Debye hypothesis we first derive the wave equations to obtain the wave velocity expression, then we derive the analytical expression of specific heat for the cubic quasicrystals and provide a set of formulas to calculate the Debye temperature Θ_D. This paper is organized as follows: In Section II based on the linear elasticity theory we derive the wave propagation equation and phase velocities for the cubic quasicrystals. In Section III, based on the results of Section II, we derive the formulas to calculate the specific heat of the cubic quasicrystals. The Section IV is a brief conclusion. Because up to now there is no related experiment dates reported yet, therefore in this article we only present the theoretical results.

LINEAR ELASTICITY THEORY AND WAVE PROPAGATION EQUATION OF THE CUBIC QUASICRYSTALS

According to the result of Wang *et al*[7], the cubic quasicrystals can be obtained by projecting a six-dimensional periodic structure onto a three-dimensional physical subspace. Letting $\vec{\xi}$ be a displacement vector in the six-dimensional space, u and w be the components of $\vec{\xi}$ in the parallel subspace (*ie*, physical subspace V_E) and perpendicular subspace (ie, complementary subspace V_I), respectively, then we have

$$\vec{\xi} = \mathrm{u} + \mathrm{w}. \qquad (1)$$

For the cubic quasicrystals which possess the crystallographic point-group symmetry, physical-property tensors in V_E and V_I can be transformed under the same irreducible representation. Therefore, they will induce the same elastic behavior in that two subspaces. If u_1, u_2, u_3 stand for the displacement components of the phonon field u, and w_1, w_2, w_3 for the displacement components of the phason field w along main-axis x_1, x_2, x_3, respectively, then we have

$$\begin{aligned} u_i &= u_i\,(x_1, x_2, x_3;\, t)\ (i = 1, 2, 3); \\ w_i &= w_i\,(x_1, x_2, x_3;\, t)\ (i = 1, 2, 3). \qquad (2) \end{aligned}$$

According to the linear elasticity theory of the cubic quasicrystals developed by Yang *et al*[8], the stress-strain relations become

$$\begin{aligned}
T_{11} &= C_{11}E_{11} + C_{12}E_{22} + C_{12}E_{33} + R_1F_{11} + R_2F_{22} + R_2F_{33} \\
T_{22} &= C_{12}E_{11} + C_{11}E_{22} + C_{12}E_{33} + R_2F_{11} + R_1F_{22} + R_2F_{33} \\
T_{33} &= C_{12}E_{11} + C_{12}E_{22} + C_{11}E_{33} + R_2F_{11} + R_2F_{22} + R_1F_{33} \\
T_{23} &= 2C_{44}E_{23} + 2R_3F_{23} = T_{32} \\
T_{31} &= 2C_{44}E_{31} + 2R_3F_{31} = T_{13} \\
T_{21} &= 2C_{44}E_{12} + 2R_3F_{12} = T_{12} \\
H_{11} &= R_1E_{11} + R_2E_{22} + R_2E_{33} + K_{11}F_{11} + K_{12}F_{22} + K_{12}F_{33} \\
H_{22} &= R_2E_{11} + R_1E_{22} + R_2E_{33} + K_{12}F_{11} + K_{11}F_{22} + K_{12}F_{33} \\
H_{33} &= R_2E_{11} + R_2E_{22} + R_1E_{33} + K_{12}F_{12} + K_{12}F_{22} + K_{11}F_{33} \\
H_{23} &= 2R_3E_{23} + 2K_{44}F_{23} = H_{32} \\
H_{31} &= 2R_3E_{31} + 2K_{44}F_{31} = H_{13} \\
H_{12} &= 2R_3E_{12} + 2K_{44}F_{12} = H_{21} \qquad (3)
\end{aligned}$$

where E_{ij} are the strain components associated with phonon field u, F_{ij} the strain components associated with phason field w and

$$E_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \quad F_{ij} = \frac{1}{2}\left(\frac{\partial w_i}{\partial x_j} + \frac{\partial w_j}{\partial x_i}\right); \quad (4)$$

T_{ij} are the stress components similar to those in conventional crystals, H_{ij} the stress components due to the existence of the phason field, C_{ij} the elastic constants of the phonon field, K_{ij} the elastic constants of the phason field, and R_i, the phonon-phason coupling elastic constants. The corresponding equations of mass-point vibration are

$$\begin{aligned}
\rho\frac{\partial^2 u_1}{\partial t^2} &= \frac{\partial T_{11}}{\partial x_1} + \frac{\partial T_{12}}{\partial x_2} + \frac{\partial T_{13}}{\partial x_3} \\
\rho\frac{\partial^2 u_2}{\partial t^2} &= \frac{\partial T_{21}}{\partial x_1} + \frac{\partial T_{22}}{\partial x_2} + \frac{\partial T_{23}}{\partial x_3} \\
\rho\frac{\partial^2 u_3}{\partial t^2} &= \frac{\partial T_{31}}{\partial x_1} + \frac{\partial T_{32}}{\partial x_2} + \frac{\partial T_{33}}{\partial x_3} \\
\rho\frac{\partial^2 w_1}{\partial t^2} &= \frac{\partial H_{11}}{\partial x_1} + \frac{\partial H_{12}}{\partial x_2} + \frac{\partial H_{13}}{\partial x_3} \\
\rho\frac{\partial^2 w_2}{\partial t^2} &= \frac{\partial H_{21}}{\partial x_1} + \frac{\partial H_{22}}{\partial x_2} + \frac{\partial H_{23}}{\partial x_3} \\
\rho\frac{\partial^2 w_3}{\partial t^2} &= \frac{\partial H_{31}}{\partial x_1} + \frac{\partial H_{32}}{\partial x_2} + \frac{\partial H_{33}}{\partial x_3} \qquad (5)
\end{aligned}$$

where ρ is the mass density of the quasicrystals. Because a cubic quasicrystal is an anisotropic crystal with nine independent elastic constants, the propagation of vibration varies with the polarization direction. In the following we first discuss the wave propagation in the direction $\wp$ of the physical space. Let l, m, n stand for the direction-cosines of $\wp$, we can rewrite the Eq (4) as follows:

$$\begin{aligned}
&E_{11} = l\frac{\partial u_1}{\partial \wp},\ E_{22} = m\frac{\partial u_2}{\partial \wp},\ E_{33} = n\frac{\partial u_3}{\partial \wp},\ E_{23} = \frac{1}{2}\left(m\frac{\partial u_2}{\partial \wp} + n\frac{\partial u_3}{\partial \wp}\right), \\
&E_{13} = \frac{1}{2}\left(n\frac{\partial u_1}{\partial \wp} + l\frac{\partial u_3}{\partial \wp}\right),\ E_{21} = \frac{1}{2}\left(l\frac{\partial u_2}{\partial \wp} + m\frac{\partial u_1}{\partial \wp}\right), \\
&F_{11} = l\frac{\partial w_1}{\partial \wp},\ F_{22} = m\frac{\partial w_2}{\partial \wp},\ F_{33} = n\frac{\partial w_3}{\partial \wp},\ F_{23} = \frac{1}{2}\left(m\frac{\partial w_2}{\partial \wp} + n\frac{\partial w_3}{\partial \wp}\right), \\
&F_{13} = \frac{1}{2}\left(n\frac{\partial w_1}{\partial \wp} + l\frac{\partial w_3}{\partial \wp}\right),\ F_{21} = \frac{1}{2}\left(l\frac{\partial w_2}{\partial \wp} + m\frac{\partial w_1}{\partial \wp}\right). \quad (6)
\end{aligned}$$

Substituting Eq (6) into Eq (3), then into Eq (5) again, we can obtain

$$\begin{aligned}
\rho\frac{\partial^2 u_1}{\partial t^2} &= \Gamma_{11}\frac{\partial^2 u_1}{\partial \wp^2} + \Gamma_{12}\frac{\partial^2 u_2}{\partial \wp^2} + \Gamma_{13}\frac{\partial^2 u_3}{\partial \wp^2} + \Gamma_{14}\frac{\partial^2 w_1}{\partial \wp^2} + \Gamma_{15}\frac{\partial^2 w_2}{\partial \wp^2} + \Gamma_{16}\frac{\partial^2 w_3}{\partial \wp^2} \\
\rho\frac{\partial^2 u_2}{\partial t^2} &= \Gamma_{21}\frac{\partial^2 u_1}{\partial \wp^2} + \Gamma_{22}\frac{\partial^2 u_2}{\partial \wp^2} + \Gamma_{23}\frac{\partial^2 u_3}{\partial \wp^2} + \Gamma_{24}\frac{\partial^2 w_1}{\partial \wp^2} + \Gamma_{25}\frac{\partial^2 w_2}{\partial \wp^2} + \Gamma_{26}\frac{\partial^2 w_3}{\partial \wp^2} \\
\rho\frac{\partial^2 u_3}{\partial t^2} &= \Gamma_{31}\frac{\partial^2 u_1}{\partial \wp^2} + \Gamma_{32}\frac{\partial^2 u_2}{\partial \wp^2} + \Gamma_{33}\frac{\partial^2 u_3}{\partial \wp^2} + \Gamma_{34}\frac{\partial^2 w_1}{\partial \wp^2} + \Gamma_{35}\frac{\partial^2 w_2}{\partial \wp^2} + \Gamma_{36}\frac{\partial^2 w_3}{\partial \wp^2} \\
\rho\frac{\partial^2 w_1}{\partial t^2} &= \Gamma_{41}\frac{\partial^2 u_1}{\partial \wp^2} + \Gamma_{42}\frac{\partial^2 u_2}{\partial \wp^2} + \Gamma_{43}\frac{\partial^2 u_3}{\partial \wp^2} + \Gamma_{44}\frac{\partial^2 w_1}{\partial \wp^2} + \Gamma_{45}\frac{\partial^2 w_2}{\partial \wp^2} + \Gamma_{46}\frac{\partial^2 w_3}{\partial \wp^2} \quad (7)
\end{aligned}$$

$$\rho\frac{\partial^2 w_2}{\partial t^2}=\Gamma_{51}\frac{\partial^2 u_1}{\partial\wp^2}+\Gamma_{52}\frac{\partial^2 u_2}{\partial\wp^2}+\Gamma_{53}\frac{\partial^2 u_3}{\partial\wp^2}+\Gamma_{54}\frac{\partial^2 w_1}{\partial\wp^2}+\Gamma_{55}\frac{\partial^2 w_2}{\partial\wp^2}+\Gamma_{56}\frac{\partial^2 w_3}{\partial\wp^2}$$

$$\rho\frac{\partial^2 w_3}{\partial t^2}=\Gamma_{61}\frac{\partial^2 u_1}{\partial\wp^2}+\Gamma_{62}\frac{\partial^2 u_2}{\partial\wp^2}+\Gamma_{63}\frac{\partial^2 u_3}{\partial\wp^2}+\Gamma_{64}\frac{\partial^2 w_1}{\partial\wp^2}+\Gamma_{65}\frac{\partial^2 w_2}{\partial\wp^2}+\Gamma_{66}\frac{\partial^2 w_3}{\partial\wp^2},$$

where

$$\begin{cases}\Gamma_{11}=C_{11}l^2+C_{44}(m^2+n^2)\\ \Gamma_{12}=C_{12}lm+C_{44}lm\\ \Gamma_{13}=C_{12}ln+C_{44}ln\\ \Gamma_{14}=R_1l^2+R_3(m^2+n^2)\\ \Gamma_{15}=R_2lm+R_3lm\\ \Gamma_{16}=R_2ln+R_3ln,\end{cases}\quad\begin{cases}\Gamma_{21}=C_{12}lm+C_{44}lm\\ \Gamma_{22}=C_{11}m^2+C_{44}(l^2+n^2)\\ \Gamma_{23}=C_{12}mn+C_{44}mn\\ \Gamma_{24}=R_2lm+R_3lm\\ \Gamma_{25}=R_1m^2+R_3(l^2+n^2)\\ \Gamma_{26}=R_2mn+R_3mn,\end{cases}\tag{8}$$

$$\begin{cases}\Gamma_{31}=C_{12}ln+C_{44}ln\\ \Gamma_{32}=C_{12}mn+C_{44}mn\\ \Gamma_{33}=C_{12}n^2+C_{44}(l^2+m^2)\\ \Gamma_{34}=R_2ln+R_3ln\\ \Gamma_{35}=R_2mn+R_3mn\\ \Gamma_{36}=R_1n^2+R_3(l^2+m^2);\end{cases}\quad\begin{cases}\Gamma_{41}=R_1l^2+R_3(m^2+n^2)\\ \Gamma_{42}=R_2lm+R_3lm\\ \Gamma_{43}=R_2ln+R_3ln\\ \Gamma_{44}=K_{11}l^2+K_{44}(m^2+n^2)\\ \Gamma_{45}=K_{12}lm+K_{44}lm\\ \Gamma_{46}=R_{12}mn+R_{44}mn,\end{cases}\tag{9}$$

$$\begin{cases}\Gamma_{51}=R_2lm+R_3lm\\ \Gamma_{52}=R_1m^2+R_3(l^2+n^2)\\ \Gamma_{53}=R_2mn+R_3mn\\ \Gamma_{54}=K_{12}lm+K_{44}lm\\ \Gamma_{55}=K_{11}m^2+K_{44}(l^2+n^2)\\ \Gamma_{56}=K_{12}mn+K_{44}mn\end{cases}\quad\begin{cases}\Gamma_{61}=R_2ln+R_3ln\\ \Gamma_{62}=R_2mn+R_3mn\\ \Gamma_{63}=R_1n^2+R_3(l^2+m^2)\\ \Gamma_{64}=K_{12}ln+K_{44}ln\\ \Gamma_{65}=K_{12}mn+K_{44}mn\\ \Gamma_{66}=K_{11}n^2+K_{44}(l^2+m^2).\end{cases}\tag{10}$$

Let $\vec{\xi}$ stand for elastic displacement vector related to the wave propagation along $\wp$ direction, and p, q, r, p', q', r' for its direction-cosines in the six-dimensional space, then

$$u_1=p\xi,\ u_2=q\xi,\ u_3=r\xi,\ w_1=p'\xi,\ w_2=q\xi,\ w_3=r\xi,$$
$$\xi=pu_1+qu_2+ru_3+p'w_1+q'w_2+r'w_3,\tag{11}$$

where ξ is the length of $\vec{\xi}$. Substituting Eq (11) into Eq (7), we obtain the following wave equation

$$p\frac{\partial^2\xi}{\partial t^2}=C^*\frac{\partial^2\xi}{\partial\wp^2},\tag{12}$$

which implies that the phase velocity $v=\sqrt{C^*/p}$, C^* is the effective elasticity coefficient, and satisfies the following equations:

$$\begin{aligned}&p\Gamma_{11}+q\Gamma_{12}+r\Gamma_{13}+p'\Gamma_{14}+q'\Gamma_{15}+r'_{16}\Gamma_{16}=pC^*\\ &p\Gamma_{21}+q\Gamma_{22}+r\Gamma_{23}+p'\Gamma_{24}+q'\Gamma_{25}+r'_{26}\Gamma_{26}=qC^*\\ &p\Gamma_{31}+q\Gamma_{32}+r\Gamma_{33}+p'\Gamma_{34}+q'\Gamma_{35}+r'_{36}\Gamma_{36}=rC^*\\ &p\Gamma_{41}+q\Gamma_{42}+r\Gamma_{43}+p'\Gamma_{44}+q'\Gamma_{45}+r'_{46}\Gamma_{46}=p'C^*\\ &p\Gamma_{51}+q\Gamma_{52}+r\Gamma_{53}+p'\Gamma_{54}+q'\Gamma_{55}+r'_{56}\Gamma_{56}=q'C^*\\ &p\Gamma_{61}+q\Gamma_{62}+r\Gamma_{63}+p'\Gamma_{64}+q'\Gamma_{65}+r'_{66}\Gamma_{66}=r'C^*.\end{aligned}\tag{13}$$

Providing that the Eq (13) has a solution, then we have

$$\begin{vmatrix}\Gamma_{11}-C^*\Gamma_{12} & \Gamma_{13} & \Gamma_{14} & \Gamma_{15} & \Gamma_{16}\\ \Gamma_{21} & \Gamma_{22}-C^* & \Gamma_{23} & \Gamma_{24} & \Gamma_{25} & \Gamma_{26}\\ \Gamma_{31}-C^*\Gamma_{32} & \Gamma_{33}-C^* & \Gamma_{34} & \Gamma_{35} & \Gamma_{36}\\ \Gamma_{41} & \Gamma_{42} & \Gamma_{43} & \Gamma_{44}-C^* & \Gamma_{45} & \Gamma_{46}\\ \Gamma_{51} & \Gamma_{52} & \Gamma_{53} & \Gamma_{54} & \Gamma_{55}-C^* & \Gamma_{56}\\ \Gamma_{61} & \Gamma_{62} & \Gamma_{63} & \Gamma_{64} & \Gamma_{65} & \Gamma_{66}-C^*\end{vmatrix}=0.\tag{14}$$

Above Eq (14) is a secular-equation of effective elastic constants C*. In principal, combining Eqs (8-10) we can solve the Eq (14) to obtain C* and then calculate the phase-velocities of wave propagation along any direction. It is however very difficult to analytically solve the Eq (14) for all propagation direction. To simplify the calculation and obtain a possible analytical solution, we consider the wave propagating along the (100) direction of cubic quasicrystals in physical subspace. In this special cace Eq (14) reduces to

$$\begin{vmatrix}C_{11}-C^* & 0 & 0 & R_1 & 0 & 0\\ 0 & C_{44}-C^* & 0 & 0 & R_3 & 0\\ 0 & 0 & C_{44}-C^* & 0 & 0 & R_3\\ R_1 & 0 & 0 & K_{11}-C^* & 0 & 0\\ 0 & R_3 & 0 & 0 & K_{44}-C^* & 0\\ 0 & 0 & R_3 & 0 & 0 & K_{44}-C^*\end{vmatrix}=0.\tag{15}$$

The solutions of above equation are, respectively,

$$C_1^* = C_4^* = \frac{1}{2}(C_{11} + K_{11}) + \frac{2R_1^2}{\sqrt{(C_{11}-K_{11})^2+4R_1^2}}, \quad (16)$$

$$C_2^* = C_3^* = C_5^* = C_6^* = \frac{1}{2}(C_{44} + K_{44}) + \frac{2R_3^2}{\sqrt{(C_{44}-K_{44})^2+4R_3^2}},$$

then the six velocities, $v_i (i = 1, \ldots 6)$, of wave propagating along the (100) direction of the cubic quasicrystals in physical-subspace have the following expressions:

$$v_1 = v_4 = \sqrt{\frac{\frac{1}{2}(C_{11} + K_{11}) + \frac{2R_1^2}{\sqrt{(C_{11}-K_{11})^2+4R_1^2}}}{\rho}}$$

$$v_2 = v_3 = v_5 = v_6 = \sqrt{\frac{\frac{1}{2}(C_{44} + K_{44}) + \frac{2R_3^2}{\sqrt{(C_{44}-K_{44})^2+4R_3^2}}}{\rho}}. \quad (17)$$

From above formulas we can see that Eq. (17) contains only four parameters C_{11}, K_{11}, R_1 and R_3. If we consider other propagation direction, says, to calculate the phase velocities of wave propagating along the (111) direction, then from Eq. (14) we will see that the velocity expression would involve nine independent elastic constants of the cubic quasicrystals. Obtaining an analytic solution is therefore very difficult. For these more general cases ones can only expect to have a numerical solution.

Specific Heat of thc Cubic Quasicrystals

After obtaining the above velocity expressions we now can evaluate the specific heat of the cubic quasicrystals by extending the Debye hypothesis to the studied systems. Debye[9] considered the crystals as a continuous elastic medium to propagate the waves of elastic vibration. Under this hypothesis he calculated the specific heat of ideal crystals, which was in good agreement with the experimental results at low temperature. We will now try to extend the Debye hypotheses to the cubic quasicrystals, i.e., we also consider the cubic quasicrystal as a continuous elastic medium. Noting that the phason do not form new degrees of freedom, the total number of freedom degrees remains three times the number of atoms contained in the cubic quasicrystal. Therefore, there are 3N independent harmonic vibration modes, where N is the number of atoms in the cubic quasicrystal. Denoting ω for the atom vibration circle-frequency and $g(\omega)$ for the frequency distribution function, then $g(\omega)d\omega$ is the number of the harmonic vibration modes between ω and $\omega + d\omega$, and we have

$$\int_0^\infty g(\omega)d\omega = 3N. \quad (18)$$

For the cubic quasicrystals containing phonon as well as phason by the Debye hypothesis we have

$$g(\omega)d\omega = B\omega^2 d\omega, \quad (19)$$

where

$$B = \frac{V}{2\pi^2}\left(\frac{1}{v_1^3} + \frac{1}{v_2^3} + \frac{1}{v_3^3} + \frac{1}{v_4^3} + \frac{1}{v_5^3} + \frac{1}{v_6^3}\right), \quad (20)$$

and V represents the volume of the cubic quasicrystals, $v_i (i = 1, \ldots, 6)$ are defined by Eq (17).

Considering that the total number of freedom degrees should be finite, so there is a maximum frequency w_D, then Eq (18) can be rewritten as

$$\int_0^{\omega_D} g(\omega)d\omega = 3N. \quad (21)$$

Substituting Eq (19) into the above formula and because the phase velocities v_i, $i = 1,2, \ldots 6$ are independent of the frequency, so we easily obtain

$$\omega_D^3 = 9N/B. \quad (22)$$

If we introduce an effective average energy , then the total energy reads

$$E = E_0 + \sum_\omega \bar{\varepsilon}(\omega) = E_0 + \int_0^{\omega_D} \bar{\varepsilon}(\omega)g(\omega)d\omega, \quad (23)$$

where E_0 is a constant and

$$\bar{\varepsilon} = \frac{\hbar\omega}{e^{\hbar\omega/kT} - 1}, \quad (24)$$

where k is the Boltzmann constant, T is the absolute temperature, respectively. According to the definition of specific heat,

$$C_V = \left(\frac{\partial E}{\partial T}\right)_V, \quad (25)$$

Using Eqs (22-24) we obtain

$$C_V = B\int_0^{\omega_D} \left(\frac{\hbar\omega}{kT}\right)^2 \frac{e^{\hbar\omega/kT} k\omega^2 d\omega}{(e^{\hbar\omega/kT}-1)^2}, \qquad (26)$$

where B is given by Eq. (20). If we introduce two new parameters x and y as following:

$$y = \frac{\hbar\omega}{kT}, \quad x = \frac{\hbar\omega_D}{kT} = \frac{\Theta_D}{T}, \qquad (27)$$

where Θ_D is the generalized Debye characteristic temperature for the cubic quasicrystals, and evaluated as

$$\Theta_D = \hbar\omega_D/k = \frac{\hbar}{k}\left(\frac{9N}{B}\right)^{1/3} = \frac{\hbar}{k}\left(\frac{18N\pi^2}{B}\right)^{1/3}\frac{1}{\chi^{1/3}} \qquad (28)$$

with

$$\chi = \left(\frac{1}{v_1^3}+\frac{1}{v_2^3}+\frac{1}{v_3^3}+\frac{1}{v_4^3}+\frac{1}{v_5^3}+\frac{1}{v_6^3}\right), \qquad (29)$$

then the Eq. (26) can be rewritten as

$$C_V = Bk\int_0^x (kT/\hbar)^3 \frac{y^4 e^y}{(e^y-1)^2}dy$$
$$= \frac{9Nk}{x^3}\int_0^x \frac{y^4 e^y}{(e^y-1)^2}dy. \qquad (30)$$

Above Eq (30) is an analytic expression of specific heat for tbe cubic quasicrystals. It is also one of the main analytic results which we expect to obtain.

Conclusion

In this paper, we first obtained the wave propagation equation of the cubic quasicrystals. Based on this equation, we derived the formulas of wave velocities propagating in the cubic quasicrystals. By extending the Debye's continuous medium hypothesis for ideal crystals to the cubic quasicrystals, we obtained the analytic expresion of specific heat for the cubic quasicrystals and provided an approach to calculate the Debye temperature Θ_D. Formally the present specific heat and Debye temperature expressions for cubic quasicrystals are almost same as that of the ideal crystals, but the Θ_D contains the contributions of the phonons, the phasons, and the coupling between phonons and phasons. Thus, the present theoretical results on the specific heat of the cubic quasicrystals are an meaningful extension of the Debye theory for ideal crystals, and also only because the special geometric structure of the cubic quasicrystals we can obtain these interesting analytical results, for other kinds of quasicrystals we generally can not obtain such impact analytical solution. Ones can only expect a numerical result, but it is a heavy and tedious work.

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On the Fourier transform of the Diamond Kernel of Marcel Riesz

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Abstract

In this paper, the operator $\diamondsuit^k$ is introduced and named as the Diamond operator iterated k-times and is defined by $\diamondsuit^k = [(\partial^2/\partial x_1^2 + \partial^2/\partial x_2^2 + \cdots + \partial^2/\partial x_p^2)^2 - (\partial^2/\partial x_{p+1}^2 + \partial^2/\partial x_{p+2}^2 + \cdots + \partial^2/\partial x_{p+q}^2)^2]^k$, where n is the dimension of the Euclidean space $\mathbb{R}^n$, k is a nonnegative integer and $p+q=n$. The elementary solution of the operator $\diamondsuit^k$ is called the Diamond Kernel of Marcel Riesz. In this work we study the Fourier transform of the elementary solution and also the Fourier transform of their convolutions.

AMS Classification: 46F10
Keywords: Diamond operator; Fourier transform; Kernel of Marcel Riesz; Dirac delta distributions; Tempered distribution

1. Introduction

Consider the equation

$$\diamondsuit^k u(x) = \delta, \tag{1}$$

where $\diamondsuit^k$ is the Diamond operator iterated k-times ($k = 0, 1, 2, \ldots$) with $\diamondsuit^0 u(x) = u(x)$ and is defined by

$$\diamondsuit^k = \left(\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \cdots + \frac{\partial^2}{\partial x_p^2}\right)^2 - \left(\frac{\partial^2}{\partial x_{p+1}^2} + \frac{\partial^2}{\partial x_{p+2}^2} + \cdots + \frac{\partial^2}{\partial x_{p+q}^2}\right)^2\right)^k, \tag{2}$$

where $p+q=n$, the dimension of the Euclidean space $\mathbb{R}^n$ and $u(x)$ is the generalized function, $x = (x_1, x_2, \ldots x_n) \in \mathbb{R}^n$ and δ is the Dirac-delta distribution.

Kananthai ([1], Theorem 1.3) has shown that the solution of convolution form $u(x) = (-1)^k S_{2k}(x) * R_{2k}(x)$ is an unique elementary solution of Eq. (1) where $S_{2k}(x)$ and $R_{2k}(x)$ are defined by Eqs. (4) and (6), respectively, with $\alpha = 2k$. Now $(-1)^k S_{2k}(x) * R_{2k}(x)$ is a generalized function, see [1], and is called the Diamond Kernel of Marcel Riesz. In this paper we study the Fourier transform of $(-1)^k S_{2k}(x) * R_{2k}(x)$ and the Fourier transform of $[(-1)^k S_{2k}(x) * R_{2k}(x)] * [(-1)^m S_{2m}(x) * R_{2m}(x)]$ where k and m are nonnegative integers.

2. Preliminaries

Definition 2.1. Let $E(x)$ be a function defined by

$$E(x) = \frac{|x|^{2-n}}{(2-n)\omega_n}, \tag{3}$$

where $x = (x_1, \dots, x_n) \in \mathbb{R}^n$, $|x| = (x_1^2 + \cdots + x_n^2)^{1/2}$ and $\omega_n = (2\pi^{n/2})/\Gamma(n/2)$ is a surface area of the unit sphere.

It is well known that $E(x)$ is an elementary solution of the Laplace operator Δ, that is $\Delta E(x) = \delta$ where $\Delta = \sum_{i=1}^n (\partial^2/\partial x_i^2)$ and δ is the Dirac-delta distribution.

Definition 2.2. Let $S_\alpha(x)$ be a function defined by

$$S_\alpha(x) = 2^{-\alpha}\pi^{-n/2}\Gamma\left(\frac{n-\alpha}{2}\right)\frac{|x|^{\alpha-n}}{\Gamma(\frac{\alpha}{2})}, \tag{4}$$

where α is a complex parameter, $|x| = (x_1^2 + \cdots + x_n^2)^{1/2}$, $x = (x_1, \dots, x_n) \in \mathbb{R}^n$.

$S_\alpha(x)$ is called the Elliptic Kernel of Marcel Riesz. Now $S_\alpha(x)$ is an ordinary function for $\mathrm{Re}(\alpha) \geqslant n$ and is a distribution of α for $\mathrm{Re}(\alpha) < n$.

From Eqs. (3) and (4) we obtain

$$E(x) = -S_2(x). \tag{5}$$

Definition 2.3. Let $x = (x_1, \dots, x_n)$ be a point in $\mathbb{R}^n$ and write

$$V = x_1^2 + x_2^2 + \cdots + x_p^2 - x_{p+1}^2 - x_{p+2}^2 - \cdots - x_{p+q}^2,$$

where $p + q = n$. Define $\Gamma_+ = \{x \in \mathbb{R}^n\colon\ x_1 > 0 \text{ and } V > 0\}$ designating the interior of the forward cone and denote $\bar{\Gamma}_+$ by its closure and the following function introduced by Nozaki ([2], p. 72),

$$R_\alpha(x) = \begin{cases} \dfrac{V^{(\alpha-n)/2}}{K_n(\alpha)}, & \text{if } x \in \Gamma_+, \\ 0, & \text{if } x \notin \Gamma_+. \end{cases} \tag{6}$$

Here $R_\alpha(x)$ is called the ultra-hyperbolic kernel of Marcel Riesz and α is a complex parameter and n is the dimension of the space $\mathbb{R}^n$.

The constant $K_n(\alpha)$ is defined by

$$K_n(\alpha) = \frac{\pi^{(n-1)/2}\Gamma(\frac{2+\alpha-n}{2})\Gamma(\frac{1-\alpha}{2})\Gamma(\alpha)}{\Gamma(\frac{2+\alpha-p}{2})\Gamma(\frac{p-\alpha}{2})}.$$

Here $R_\alpha(x)$ is an ordinary function if $\mathrm{Re}(\alpha) \geqslant n$ and is a distribution of α if $\mathrm{Re}(\alpha) < n$.

Let $\operatorname{supp} R_\alpha(x) \subset \bar{\Gamma}_+$ where $\operatorname{supp} R_\alpha(x)$ denote the support of $R_\alpha(x)$.

Definition 2.4. Let f be a continuous function, the Fourier transform of f denoted by

$$\mathscr{F}f = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-i\xi x}\, dx, \tag{7}$$

where $x = (x_1, \ldots, x_n) \in \mathbb{R}^n, \xi = (\xi_1, \ldots, \xi_n) \in \mathbb{R}^n$ and $\xi x = \xi_1 x_1 + \xi_2 x_2 + \cdots + \xi_n x_n$. Sometimes we write $\mathscr{F}f(x) \equiv \hat{f}(\xi)$. By Eq. (7), we can define the inverse of the Fourier transform of $\hat{f}(\xi)$ by

$$f(x) = \mathscr{F}^{-1}\hat{f}(\xi) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}} e^{i\xi x}\hat{f}(\xi)\, d\xi. \tag{8}$$

If f is a distribution with compact supports by [3], Theorem 7.4-3, p. 187 Eq. (7) can be written as

$$\mathscr{F}f = \frac{1}{(2\pi)^{n/2}} \langle f(x), e^{-i\xi x}\rangle. \tag{9}$$

Lemma 2.1. *The functions $S_\alpha(x)$ and $R_\alpha(x)$ defined by Eqs. (4) and (6), respectively, for $\mathrm{Re}(\alpha) < n$ are homogeneous distributions of order $\alpha - n$.*

Proof. Since $R_\alpha(x)$ and $S_\alpha(x)$ satisfy the Euler equation, that is

$$(\alpha - n)R_\alpha(x) = \sum_{i=1}^{n} x_i \frac{\partial}{\partial x_i} R_\alpha(x) \text{ and } (\alpha - n)S_\alpha(x) = \sum_{i=1}^{n} x_i \frac{\partial}{\partial x_i} S_\alpha(x),$$

we have that $R_\alpha(x)$ and $S_\alpha(x)$ are homogeneous distributions of order $\alpha - n$.

Donoghue ([4], pp. 154 and 155) has proved that every homogeneous distribution is a tempered distribution.

That completes the proof.

Lemma 2.2 (The convolution of tempered distributions). *The convolution $S_\alpha(x) * R_\alpha(x)$ exists and is a tempered distribution.*

Proof. Choose supp $R_\alpha(x) = K \subset \bar{\Gamma}_+$ where K is a compact set. Then $R_\alpha(x)$ is a tempered distribution with compact support and by [3], pp. 156–159 $S_\alpha(x) * R_\alpha(x)$ exists and is a tempered distribution.

Lemma 2.3. *Given the equation* $\diamondsuit^k u(x) = \delta$ *where the operator* $\diamondsuit^k$ *is defined by Eq. (2),* $x = (x_1, \ldots, x_n) \in \mathbb{R}^n$, k *is a nonnegative integer and* δ *is the Dirac-delta distribution, then* $u(x) = (-1)^k S_{2k}(x) * R_{2k}(x)$ *is the unique elementary solution of the equation where* $S_{2k}(x)$ *and* $R_{2k}(x)$ *are defined by Eqs. (4) and (6), respectively, with* $\alpha = 2k$.

Proof. By Lemma 2.2, for $\alpha = 2k$, the distribution $(-1)^k S_{2k}(x) * R_{2k}(x)$ exists and is a tempered distribution.

Now the distribution $(-1)^k S_{2k}(x)$ is obtained by the convolution

$$\underbrace{E(x) * E(x) * \cdots * E(x)}_{k\text{-times}} = \underbrace{(-S_2(x)) * (-S_2(x)) * \cdots * (-S_2(x))}_{k\text{-times}},$$

where $E(x)$ is defined by Eq. (3) and by Eq. (5).

Kananthai ([5], Lemma 2.5) has shown that

$$\underbrace{-S_2(x) * (-S_2(x)) * \cdots * (-S_2(x))}_{k\text{-times}} = (-1)^k S_{2k}(x)$$

is an elementary solution of the Laplace operator Δ^k iterated k-times. By Eq. (2), $\diamondsuit^k$ can be written as

$$\diamondsuit^k = \square^k \Delta^k, \tag{10}$$

where

$$\square^k = \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \cdots + \frac{\partial^2}{\partial x_p^2} - \frac{\partial^2}{\partial x_{p+1}^2} - \cdots - \frac{\partial^2}{\partial^2_{p+q}} \right)^k$$

and

$$\Delta^k = \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \cdots + \frac{\partial^2}{\partial x_n^2} \right)^k, \quad p + q = n.$$

By [1], Theorem 3.1 $u(x) = (-1)^k S_{2k}(x) * R_{2k}(x)$ is the unique elementary solution of the operator $\diamondsuit^k$ as required.

Lemma 2.4 (The Fourier transform of $\diamondsuit^k \delta$).

$$\mathscr{F} \diamondsuit^k \delta = \frac{1}{(2\pi)^{n/2}} \left((\xi_1^2 + \xi_2^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \xi_{p+2}^2 + \cdots + \xi_{p+q}^2)^2 \right)^k,$$

where $\mathscr{F}$ is the Fourier transform defined by Eq. (7) and if the norm of ξ is given by $\|\xi\| = (\xi_1^2 + \xi_2^2 + \cdots + \xi_n^2)^{1/2}$ then

$$|\mathscr{F}\Diamond^k\delta| \leqslant \frac{1}{(2\pi)^{n/2}}\|\xi\|^{4k} \tag{11}$$

that is $\mathscr{F}\Diamond^k\delta$ is bounded and continuous on the space S' of the tempered distribution. Moreover, by Eq. (8)

$$\Diamond^k\delta = \mathscr{F}^{-1}\frac{1}{(2\pi)^{n/2}}\left((\xi_1^2 + \xi_2^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \xi_{p+2}^2 + \cdots + \xi_{p+q}^2)^2\right)^k.$$

Proof. By Eq. (9)

$$\begin{aligned}
\mathscr{F}\Diamond^k\delta &= \frac{1}{(2\pi)^{n/2}}\langle\Diamond^k\delta, e^{-i\xi x}\rangle \\
&= \frac{1}{(2\pi)^{n/2}}\langle\delta, \Diamond^k e^{-i\xi x}\rangle \\
&= \frac{1}{(2\pi)^{n/2}}\langle\delta, \Box^k\Delta^k e^{-i\xi x}\rangle \quad \text{by (10)} \\
&= \frac{1}{(2\pi)^{n/2}}\langle\delta, (-1)^k(\xi_1^2 + \xi_2^2 + \cdots + \xi_n^2)^k\Box^k e^{-i\xi x}\rangle \\
&= \frac{1}{(2\pi)^{n/2}}\langle\delta, (-1)^k(\xi_1^2 + \xi_2^2 + \cdots + \xi_n^2)^k(-1)^k \\
&\quad \times (\xi_1^2 + \xi_2^2 + \cdots + \xi_p^2 - \xi_{p+1}^2 - \xi_{p+2}^2 - \cdots - \xi_{p+2}^2)^k e^{-i\xi x}\rangle \\
&= \frac{1}{(2\pi)^{n/2}}(-1)^{2k}((\xi_1^2 + \cdots + \xi_n^2)^k \times (\xi_1^2 + \cdots + \xi_p^2 - \xi_{p+1}^2 - \cdots - \xi_{p+q}^2)^k \\
&= \frac{1}{(2\pi)^{n/2}}\left((\xi_1^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \cdots + \xi_{p+q}^2)^2\right)^k.
\end{aligned}$$

Now

$$\begin{aligned}
|\mathscr{F}\Diamond^k\delta| &= \frac{1}{(2\pi)^{n/2}}\left(|\xi_1^2 + \cdots + \xi_n^2||\xi_1^2 + \cdots + \xi_p^2 - \xi_{p+1}^2 - \cdots \xi_{p+q}^2|\right)^k \\
&\leqslant \frac{1}{(2\pi)^{n/2}}\left(|\xi_1^2 + \cdots + \xi_n^2|\right)^k \\
&= \frac{1}{(2\pi)^{n/2}}\|\xi\|^{4k},
\end{aligned}$$

where $\|\xi\| = (\xi_1^2 + \cdots + \xi_n^2)^{1/2}$, $\xi_i\ (i = 1, 2, \ldots, n) \in \mathbb{R}$. Hence we obtain Eq. (11) and $\mathscr{F}\Diamond^k\delta$ is bounded and continuous on the space S' of the tempered distribution.

Since $\mathscr{F}$ is 1–1 transformation from the space S' of the tempered distribution to the real space R, then by Eq. (8)

$$\Diamond^k \delta = \frac{1}{(2\pi)^{n/2}} \mathscr{F}^{-1}\left((\xi_1^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \cdots + \xi_{p+q}^2)^2\right)^k.$$

That completes the proof.

3. Main results

Theorem 3.1.

$$\mathscr{F}((-1)^k S_{2k}(x) * R_{2k}(x)) = \frac{1}{(2\pi)^{n/2}[(\xi_1^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \cdots + \xi_{p+q}^2)^2]^k}$$

and

$$|\mathscr{F}((-1)^k S_{2k}(x) * R_{2k}(x))| \leqslant \frac{1}{(2\pi)^{n/2}} M \text{ for a large } \xi_i \in R, \tag{12}$$

where M is a constant. That is $\mathscr{F}$ is bounded and continuous on the space S' of the tempered distributions.

Proof. By Lemma 2.3 $\Diamond^k((-1)^k S_{2k}(x) * R_{2k}(x) = \delta$ or $(\Diamond^k \delta) * [(-1)^k S_{2k}(x) * R_{2k}(x)] = \delta$.

Taking the Fourier transform on both sides, we obtain

$$\mathscr{F}((\Diamond^k \delta) * [(-1)^k S_{2k}(x) * R_{2k}(x)]) = \mathscr{F}\delta = \frac{1}{(2\pi)^{n/2}}.$$

By Eq. (9)

$$\frac{1}{(2\pi)^{n/2}} \langle (\Diamond^k \delta) * [(-1)^k S_{2k}(x) * R_{2k}(x)], e^{-i\xi x} \rangle = \frac{1}{(2\pi)^{n/2}}.$$

By the definition of convolution

$$\frac{1}{(2\pi)^{n/2}} \langle (\Diamond^k \delta), \langle [(-1)^k S_{2k}(r) * R_{2k}(r)], e^{-i\xi(x+r)} \rangle \rangle = \frac{1}{(2\pi)^{n/2}},$$

$$\frac{1}{(2\pi)^{n/2}} \langle [(-1)^k S_{2k}(r) * R_{2k}(r)], e^{-i\xi r} \rangle \langle (\Diamond^k \delta), e^{-i\xi x} \rangle = \frac{1}{(2\pi)^{n/2}},$$

$$\mathscr{F}([(-1)^k S_{2k}(r) * R_{2k}(r)])(2\pi)^{n/2} \mathscr{F}(\Diamond^k \delta) = \frac{1}{(2\pi)^{n/2}}.$$

By Lemma 2.4,

$$\mathscr{F}([(-1)^k S_{2k}(x) * R_{2k}(x)])((\xi_1^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \cdots + \xi_{p+q}^2)^2)^k = \frac{1}{(2\pi)^{n/2}}.$$

It follows that

$$\mathscr{F}([(-1)^k S_{2k}(x) * R_{2k}(x)]) = \frac{1}{(2\pi)^{n/2}[(\xi_1^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \cdots + \xi_{p+q}^2)^2]^k}.$$

Now

$$\begin{aligned} &\frac{1}{[(\xi_1^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \cdots + \xi_{p+q}^2)^2]^k} \\ &\quad = \frac{1}{(\xi_1^2 + \cdots + \xi_n^2)^k} \frac{1}{(\xi_1^2 + \cdots + \xi_p^2 - \xi_{p+1}^2 - \cdots - \xi_{p+q}^2)^k}. \end{aligned} \tag{13}$$

Let $\xi = (\xi_1, \ldots, \xi_n) \in \Gamma_+$ with Γ_+ defined by Definition 2.3. Then $(\xi_1^2 + \cdots + \xi_p^2 - \xi_{p+1}^2 - \cdots - \xi_{p+q}^2) > 0$ and for a large ξ_i and a large k, the right-hand side of Eq. (13) tends to zero. It follows that it is bounded by a positive constant M say, that is we obtain Eq. (12) as required and also by Eq. (12) $\mathscr{F}$ is continuous on the space S' of the tempered distribution.

Theorem 3.2.

$$\begin{aligned} &\mathscr{F}([(-1)^k S_{2k}(x) * R_{2k}(x)] * [(-1)^m S_{2m}(x) * R_{2m}(x)]) \\ &\quad = (2\pi)^{n/2} \mathscr{F}([(-1)^k S_{2k}(x) * R_{2k}(x)] \mathscr{F}[(-1)^m S_{2m}(x) * R_{2m}(x)] \\ &\quad = \frac{1}{(2\pi)^{n/2}} \frac{1}{[(\xi_1^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \cdots + \xi_{p+q}^2)^2]^{k+m}}, \end{aligned}$$

where k and m are nonnegative integers and $\mathscr{F}$ is bounded and continuous on the space S' of the tempered distribution.

Proof. Since $R_{2k}(x)$ and $S_{2k}(x)$ are tempered distributions with compact supports, we have

$$\begin{aligned} &[(-1)^k S_{2k}(x) * R_{2k}(x)] * [(-1)^m S_{2m}(x) * R_{2m}(x)] \\ &\quad = (-1)^{k+m}(S_{2k}(x) * S_{2m}(x)) * (R_{2k}(x) * R_{2m}(x)) \\ &\quad = (-1)^{k+m}(S_{2(k+m)}(x) * R_{2(k+m)}(x)) \end{aligned}$$

by [3], pp. 156–159 and [2], Lemma 2.5. Taking the Fourier transform on both sides and using Theorem 3.1 we obtain

$$
\begin{aligned}
&\mathscr{F}([(-1)^k S_{2k}(x) * R_{2k}(x)] * [(-1)^m S_{2m}(x) * R_{2m}(x)]) \\
&= \frac{1}{(2\pi)^{n/2}((\xi_1^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \cdots + \xi_{p+q}^2)^2)^{k+m}} \\
&= \frac{1}{(2\pi)^{n/2}((\xi_1^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \cdots + \xi_{p+q}^2)^2)^{k}} \\
&\quad \times \frac{(2\pi)^{n/2}}{(2\pi)^{n/2}((\xi_1^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \cdots + \xi_{p+q}^2)^2)^{m}} \\
&= (2\pi)^{n/2} \mathscr{F}[(-1)^k S_{2k}(x) * R_{2k}(x)] \mathscr{F}[(-1)^m S_{2m}(x) * R_{2m}(x)].
\end{aligned}
$$

Since $(-1)^k S_{2(k+m)}(x) * R_{2(k+m)}(x) \in S'$, the space of tempered distribution, and by Theorem 3.1 we obtain that $\mathscr{F}$ is bounded and continuous on S'.

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On the convolutions of the diamond kernel of Marcel Riesz

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Abstract

In this paper, we consider the equation $\diamondsuit^k u(x) = \delta$ where $\diamondsuit^k$ is introduced and named as the diamond operator iterated k-times and is defined by $\diamondsuit^k = ((\sum_{i=1}^{p}(\partial^2/\partial x_i^2))^2 - (\sum_{j=p+1}^{p+q}(\partial^2/\partial x_j^2))^2)^k$, $u(x)$ is a generalized function, $x = (x_1, x_2, \ldots, x_n) \in R^n$ the n-dimensional Euclidean space, $p + q = n$, $k = 0, 1, 2, 3, \ldots$ and δ is the Dirac-delta distribution. Now $u(x)$ is the elementary solution of the operator $\diamondsuit^k$ and is called the diamond kernel of Marcel Riesz. The main part of this work is studying the convolution of $u(x)$.

Keywords: Diamond kernel; Ultra-hyperbolic kernel; Elliptic kernel; Tempered distribution

1. Introduction

Consider the equation

$$\diamondsuit^k u(x) = \delta, \tag{1.1}$$

where $\diamondsuit^k$ is the Diamond operator iterated k-times defined by

$$\diamondsuit^k = \left(\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \cdots + \frac{\partial^2}{\partial x_p^2}\right)^2 - \left(\frac{\partial^2}{\partial x_{p+1}^2} + \frac{\partial^2}{\partial x_{p+2}^2} + \cdots + \frac{\partial^2}{\partial x_{p+q}^2}\right)^2\right)^k. \tag{1.2}$$

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Kananthai [2, Theorem 3.1] has proved that the convolution solution $u(x) = (-1)^k S_{2k}(x) * R_{2k}(x)$ is the elementary solution of (1.1) where $S_{2k}(x)$ and $R_{2k}(x)$ are defined by (2.2) and (2.4), respectively with $\alpha = 2k$. Now $u(x)$ is called the diamond kernel of Marcel Riesz and defines such a kernel by

$$T_m(x) = (-1)^m S_{2m}(x) * R_{2m}(x), \quad m = 0, 1, 2, \ldots \tag{1.3}$$

In this work we study the existence of $T_m(x) * T_n(x)$ and moreover the inverse T_m^{*-1} of $T_m(x)$ in the convolution algebra $\mathscr{A}'$ is also considered.

2. Preliminaries

Definition 2.1. Let $E(x)$ be a function defined by

$$E(x) = \frac{|x|^{2-n}}{(2-n)\omega_n}, \tag{2.1}$$

where $x = (x_1, x_2, \ldots, x_n) \in R^n$, $|x| = (x_1^2 + x_2^2 + \cdots + x_n^2)^{1/2}$ and $\omega_n = (2\pi^{n/2})/(\Gamma(n/2))$ is a surface area of the unit sphere.

It is well known that $E(x)$ is an elementary solution of the Laplace operator Δ, that $\Delta E(x) = \delta$ where $\Delta = \sum_{i=1}^n \partial^2/\partial x_i^2$ and δ is the Dirac-delta distribution.

Definition 2.2. Let $S_\alpha(x)$ be a function defined by

$$S_\alpha(x) = 2^{-\alpha}\pi^{-n/2}\Gamma\left(\frac{n-\alpha}{2}\right)\frac{|x|^{\alpha-n}}{\Gamma(\alpha/2)}, \tag{2.2}$$

where α is a complex parameter, $|x| = (x_1^2 + x_2^2 + \cdots + x_n^2)^{1/2}$, $x = (x_1, x_2, \ldots, x_n) \in R^n$. $S_\alpha(x)$ is called the elliptic kernel of Marcel Riesz. Now $S_\alpha(x)$ is an ordinary function for $\mathrm{Re}(\alpha) \geqslant n$ and is a distribution of α for $\mathrm{Re}(\alpha) < n$.

From (2.1) and (2.2) we obtain

$$E(x) = -S_2(x) \tag{2.3}$$

and it can be shown that

$$\underbrace{E(x) * E(x) * \cdots * E(x)}_{k\text{-times}} = (-1)^k S_{2k}(x)$$

is the elementary solution of the operator Δ^k iterated k-times that is $\Delta^k(-1)^k S_{2k}(x) = \delta$, see [3].

Definition 2.3. Let $x = (x_1, x_2, \ldots, x_n)$ be a point of R^n and write

$$V = x_1^2 + x_2^2 + \cdots + x_p^2 - x_{p+1}^2 - x_{p+2}^2 - \cdots - x_{p+q}^2, \quad p + q = n.$$

$\Gamma_+ = \{x \in R^n : x_1 > 0 \text{ and } V > 0\}$ designates the interior of the forward cone and denotes $\overline{\Gamma}_+$ by its closure and the following function introduced by Nozaki [4, p. 72] that

$$R_\alpha(x) = \begin{cases} V^{(\alpha-n)/2}/K_n(\alpha) & \text{if } x \in \Gamma_+, \\ 0 & \text{if } x \notin \Gamma_+. \end{cases} \tag{2.4}$$

Here, $R_\alpha(x)$ is called the ultra-hyperbolic kernel of Marcel Riesz and α is a complex parameter and n is the dimension of the space R^n.

The constant $K_n(\alpha)$ is defined by

$$K_n(\alpha) = \frac{\pi^{(n-1)/2}\Gamma((2+\alpha-n)/2)\Gamma((1-\alpha)/2)\Gamma(\alpha)}{\Gamma((2+\alpha-p)/2)\Gamma((p-\alpha)/2)}.$$

Now $R_\alpha(x)$ is an ordinary function if $\mathrm{Re}(\alpha) \geqslant n$ and is a distribution of α if $\mathrm{Re}(\alpha) < n$.

Let $\operatorname{supp} R_\alpha(x) \subset \overline{\Gamma}_+$ where $\operatorname{supp} R_\alpha(x)$ denotes the support of $R_\alpha(x)$.

Lemma 2.1. *The functions $S_\alpha(n)$ and $R_\alpha(x)$ defined by* (2.2) *and* (2.4) *respectively, for* $\mathrm{Re}(\alpha) < n$ *are Homogeneous distribution of order $\alpha - n$ and also a tempered distribution.*

Proof. Since $R_\alpha(x)$ and $S_\alpha(x)$ satisfy the Euler equation, that is

$$(\alpha - n)R_\alpha(x) = \sum_{i=1}^{n} x_i \frac{\partial}{\partial x_i} S_\alpha(x) \quad \text{and} \quad (\alpha - n)S_\alpha(x) = \sum_{i=1}^{n} x_i \frac{\partial}{\partial x_i} R_\alpha(x),$$

we have $R_\alpha(x)$ and $S_\alpha(x)$ are homogeneous distributions of order $\alpha - n$ and Donoghue [1, pp. 154–155] has proved that every homogeneous distribution is a tempered distribution. That completes the proof. □

Lemma 2.2 (The convolution of tempered distributions). *The convolution $S_\alpha(x) * R_\alpha(x)$ exists and is a tempered distribution.*

Proof. Choose $\operatorname{supp} R_\alpha(x) = K \subset \overline{\Gamma}_+$ where K is a compact set. Then $R_\alpha(x)$ is a tempered distribution with compact support and by Donoghue [1, pp. 156–159], $S_\alpha(x) * R_\alpha(x)$ exists and is a tempered distribution. □

Lemma 2.3. *Given the equation $\diamondsuit^k u(x) = \delta$ where $\diamondsuit^k$ is the operator defined by* (1.2), $x = (x_1, x_2, \ldots, x_n) \in R^n$, *$K$ is a nonnegative integer and δ is the Dirac-delta distribution. Then $u(x) = (-1)^k S_{2k}(x) * R_{2k}(x)$ is the unique elementary solution of the equation where $S_\alpha(x)$ and $R_\alpha(x)$ are defined by* (2.2) *and* (2.4), *respectively with $\alpha = 2k$. Moreover $u(x)$ is a tempered distribution.*

Proof. See [3, Theorem 3.1] and by Lemma 2.2, $u(x) = (-1)^k S_{2k}(x) * R_{2k}(x)$ is a tempered distribution. $\square$

Lemma 2.4 (The convolutions of $R_\alpha(x)$ and $S_\alpha(x)$). *Let $S_\alpha(x)$ and $R_\alpha(x)$ be defined by* (2.2) *and* (2.4) *respectively, then we obtain the following formulas*:
1. $S_\alpha(x) * S_\beta(x) = S_{\alpha+\beta}(x)$, *where α and β are complex parameters.*
2. $R_\alpha(x) * R_\beta(x) = R_{\alpha+\beta}(x)$, *for α and β are both integers and except only the case both α and β are odd integers.*

Proof. Proof of first formula, see [1, p. 158].

Proof of second formula, for the case α and β are both even integers, see [3] and for the case α is odd and β is even or α is even and β is odd, we know from Trione [5] that

$$\square^k R_\alpha(x) = R_{\alpha-2k}(x) \tag{2.5}$$

and

$$\square^k R_{2k} = \delta, \quad k = 0, 1, 2, \ldots \tag{2.6}$$

where $\square^k$ is and ultra-hyperbolic operator iterated k-times $(k = 0, 1, 2, \ldots)$ defined by

$$\square^k = \left(\sum_{i=1}^{p} \frac{\partial^2}{\partial x_i^2} - \sum_{j=p+1}^{p+q} \frac{\partial^2}{\partial x_j^2} \right)^k .$$

Now let m be an odd integer, we have

$$\square^k R_m(x) = R_{m-2k}(x)$$

and

$$R_{2k}(x) * \square^k R_m(x) = R_{2k}(x) * R_{m-2k}(x)$$

or

$$(\square^k R_{2k}(x)) * R_m(x) = R_{2k}(x) * R_{m-2k}(x),$$

$$\delta * R_m(x) = R_{2k}(x) * R_{m-2k}(x) \quad \text{by (2.6)},$$

or

$$R_m(x) = R_{2k}(x) * R_{m-2k}(x).$$

Since m is odd, hence $m - 2k$ is odd and $2k$ is a positive even. Put $\alpha = 2k$, $\beta = m - 2k$ we obtain

$$R_\alpha(x) * R_\beta(x) = R_{\alpha+\beta}(x)$$

for α is a nonnegative even and β is odd.

For the case α is a negative even and β is odd, by (2.5) we have

$$\Box^k R_0(x) = R_{-2k}(x) \quad \text{or} \quad \Box^k \delta = R_{-2k}(x)$$

where $R_0(x) = \delta$. Now

$$R_{-2k}(x) * \Box^k R_m(x) = R_{-2k}(x) * R_{m-2k}(x) \quad \text{for } m \text{ is odd,}$$

or

$$(\Box^k \delta) * \Box^k R_m(x) = R_{-2k}(x) * R_{m-2k}(x),$$

$$\delta * \Box^{2k} R_m(x) = R_{-2k}(x) * R_{m-2k}(x),$$

$$R_{m-2(2k)}(x) = R_{-2k}(x) * R_{m-2k}(x).$$

Put $\alpha = -2k$ and $\beta = m - 2k$, now α is a negative even and β is odd. Then we obtain

$$R_\alpha(x) * R_\beta(x) = R_{\alpha+\beta}(x).$$

That completes the proofs. $\Box$

3. Main results

Theorem 3.1. *Let $T_m(x)$ the diamond kernel of Marcel Riesz defined by* (1.3), *then T_m is a tempered distribution and can be expressed by*

$$T_m(x) = T_{m-r}(x) * T_r(x),$$

where r is a nonnegative integer and $r < m$. Moreover if we put $\ell = m - r,\ n = r$ we obtain

$$T_\ell(x) * T_n(x) = T_{\ell+n}(x) \quad \textit{for } \ell + n = m.$$

Proof. Since $T_m = (-1)^m S_{2m}(x) * R_{2m}(x),\ (m = 0, 1, 2, \ldots)$, by Lemma 2.2 T_m is a tempered distribution. Now by Lemma 2.3, $\Diamond^m T_m = \delta$, then $\Diamond^r \Diamond^{m-r} T_m = \delta$ for $m > r$ and by Lemma 2.3 again, we obtain $\Diamond^{m-r} T_m = (-1)^r S_2 r(x) * R_{2r}(x)$. Convolving both sides by $(-1)^{m-r} S_{2(m-r)}(x) * R_{2(m-r)}(x)$, we obtain

$$\begin{aligned}&[(-1)^{m-r} S_{2(m-r)}(x) * R_{2(m-r)}(x)] * \Diamond^{m-r} T_m \\ &\quad = [(-1)^{m-r} S_{2m-2r}(x) * R_{2m-2r}(x)] * [(-1)^r S_{2r}(x) * R_{2r}(x)]\end{aligned} \tag{3.1}$$

or

$$\begin{aligned}&\Diamond^{m-r}[(-1)^{m-r} S_{2(m-r)}(x) * R_{2(m-r)}(x)] * T_m \\ &\quad = (-1)^m (S_{2m-2r}(x) * S_{2r}(x) * (R_{2m-2r}(x) * R_{2r}(x)),\end{aligned}$$

since $S_{2m}(x)$ and $R_{2m}(x)$ are tempered distributions and are the elements of the space of convolution algebra, $\mathscr{a}'$.

By Lemmas 2.3 and 2.4 we obtain

$$\delta * T_m(x) = (-1)^m S_{2m}(x) * R_{2m}(x),$$
$$T_m(x) = (-1)^m S_{2m}(x) * R_{2m}(x).$$

From (3.1) we have $T_m(x) = T_{m-r}(x) * T_r(x)$, put $\ell = m - r$, $n = r$, it follows that

$$T_\ell(x) * T_n(x) = T_{\ell+n}(x) = T_m(x)$$

as required. □

Theorem 3.2. *Let $T_m(x)$ be defined by* (1.3) *then T_m is an element of the space $\mathscr{a}'$ of convolution algebra and there exist an inverse T_m^{*-1} of T_m such that*

$$T_m(x) * T_m^{*-1} = T_m^{*-1} * T_m(x) = \delta.$$

Proof. Since $T_m(x) = (-1)^m S_{2m}(x) * R_{2m}(x)$ is a tempered distribution by Lemma 2.2. Now the supports of $S_{2m}(x)$ and $R_{2m}(x)$ are compact. Then they are the elements of the space of convolution algebra $\mathscr{a}'$ of distribution. By Zemanian [6, Theorem 6.2.1, p. 151] there exist a unique inverse T_m^{*-1} such that

$$T_m(x) * T_m^{*-1} = T_m^{*-1} * T_m(x) = \delta.$$

That completes the proof. □

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ON THE SPECTRUM OF THE DISTRIBUTIONAL KERNEL RELATED TO THE RESIDUE

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ABSTRACT. We study the spectrum of the distributional kernel $K_{\alpha,\beta}(x)$, where α and β are complex numbers and x is a point in the space $\mathbb{R}^n$ of the n-dimensional Euclidean space. We found that for any nonzero point ξ that belongs to such a spectrum, there exists the residue of the Fourier transform $(-1)^k\widehat{K_{2k,2k}(\xi)}$, where $\alpha = \beta = 2k$, k is a nonnegative integer and $\xi \in \mathbb{R}^n$.

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1. Introduction. Gel'fand and Shilov [2, pages 253–256] have studied the generalized function P^λ, where

$$P = \sum_{i=1}^{p} x_i^2 - \sum_{j=p+1}^{p+q} x_j^2 \tag{1.1}$$

is a quadratic form, λ is a complex number, and $p+q=n$ is the dimension of $\mathbb{R}^n$. They found that P^λ has two sets of singularities, namely $\lambda = -1,-2,\dots,-k,\dots$ and $\lambda = -n/2,-n/2-1,\dots,-n/2-k,\dots$, where k is a positive integer. For the singular point $\lambda = -k$, the generalized function P^λ has a simple pole with residue

$$\frac{(-1)^k}{(k-1)!}\delta_1^{(k-1)}(P) \quad \text{or} \quad \operatorname{res}_{\lambda=-k} P^\lambda = \frac{(-1)^k}{(k-1)!}\delta_1^{(k-1)}(P) \tag{1.2}$$

for $p+q=n$ is odd with p odd and q even. Also, for the singular point $\lambda = -n/2-k$ they obtained

$$\operatorname{res}_{\lambda=-n/2-k} P^\lambda = \frac{(-1)^{q/2}L^k\delta(x)}{2^{2k}k!\Gamma((n/2)+k)} \tag{1.3}$$

for $p+q=n$ is odd with p odd and q even.

Now, let $K_{\alpha,\beta}(x)$ be the convolution of the functions $R_\alpha^H(u)$ and $R_\beta^\ell(v)$, that is,

$$K_{\alpha,\beta}(x) = R_\alpha^H(u) * R_\beta^\ell(v), \tag{1.4}$$

where $R_\alpha^H(u)$ and $R_\beta^\ell(v)$ are defined by (2.1) and (2.3), respectively. Since $R_\alpha^H(u)$ and $R_\beta^\ell(v)$ are tempered distributions, see [4, pages 30-31], thus $K_{\alpha,\beta}(x)$ is also a tempered distribution and is called the distributional kernel.

In this paper, we use the idea of Gel'fand and Shilov to find the residue of the Fourier transform $(-1)^k\widehat{K_{2k,2k}(\xi)}$, where $K_{2k,2k}$ is defined by (1.4) with $\alpha=\beta=2k$ and k is a nonnegative integer. We found that for any nonzero point ξ that belongs to the spectrum of $(-1)^kK_{2k,2k}(x)$, there exists the residue of the Fourier transform

$(-1)^k\widehat{K_{2k,2k}(\xi)}$. Actually $(-1)^k K_{2k,2k}(x)$ is an elementary solution of the operator $\diamond^k$ iterated k times, that is, $\diamond^k[(-1)^k K_{2k,2k}(x)] = \delta$, where δ is the Dirac-delta distribution.

The operator $\diamond^k$ was first introduced by Kananthai [4] and named as the Diamond operator defined by

$$\diamond^k = \left[\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \cdots + \frac{\partial^2}{\partial x_p^2}\right)^2 - \left(\frac{\partial^2}{\partial x_{p+1}^2} + \frac{\partial^2}{\partial x_{p+2}^2} + \cdots + \frac{\partial^2}{\partial x_{p+q}^2}\right)^2\right]^k, \tag{1.5}$$

where $p+q=n$ is the dimension of $\mathbb{R}^n$.

Moreover, the operator $\diamond^k$ can be expressed as the product of the operators $\Box^k$ and $\triangle^k$, that is,

$$\diamond^k = \Box^k \triangle^k = \triangle^k \Box^k, \tag{1.6}$$

where $\Box^k$ is an ultra-hyperbolic operator iterated k times defined by

$$\Box^k = \left(\sum_{i=1}^{p} \frac{\partial^2}{\partial x_i^2} - \sum_{j=p+1}^{p+q} \frac{\partial^2}{\partial x_j^2}\right)^k, \tag{1.7}$$

where $p+q=n$. The operator $\triangle^k$ is an elliptic operator or Laplacian iterated k times defined by

$$\triangle^k = \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \cdots + \frac{\partial^2}{\partial x_n^2}\right)^k. \tag{1.8}$$

Trione [7, page 11] has shown that the function $R_{2k}^H(u)$ defined by (2.1) with $\alpha = 2k$ is an elementary solution of the operator $\Box^k$. Also, Aguirre Téllez [1, pages 147-148] has proved that the solution $R_{2k}^H(u)$ exists only for odd n with p odd and q even $(p+q=n)$. Moreover, we can show that the function $(-1)^k R_{2k}^{\ell}(v)$ is an elementary solution of the operator $\triangle^k$, where $R_{2k}^{\ell}(v)$ is defined by (2.3) with $\beta = 2k$.

2. Preliminaries

Definition 2.1. Let $x = (x_1, x_2, \ldots, x_n)$ be a point of $\mathbb{R}^n$, and write $u = x_1^2 + x_2^2 + \cdots + x_p^2 - x_{p+1}^2 - \cdots - x_{p+q}^2$, $p+q=n$. Denote by $\Gamma_+ = \{x \in \mathbb{R}^n : x_1 > 0,\ u > 0\}$ the set of an interior of the forward cone, and $\overline{\Gamma_+}$ denotes the closure of Γ_+. For any complex number α, define

$$R_\alpha^H(u) = \begin{cases} \dfrac{u^{(\alpha-n)/2}}{K_n(\alpha)}, & \text{for } x \in \Gamma_+, \\ 0, & \text{for } x \notin \Gamma_+, \end{cases} \tag{2.1}$$

where the constant $K_n(\alpha)$ is given by the formula

$$K_n(\alpha) = \frac{\pi^{(n-1)/2}\Gamma((2+\alpha-n)/2)\Gamma((1-\alpha)/2)\Gamma(\alpha)}{\Gamma((2+\alpha-p)/2)\Gamma((p-\alpha)/2)}. \tag{2.2}$$

The function $R_\alpha^H(u)$ is called the ultra-hyperbolic kernel of Marcel Riesz and was introduced by Nozaki [6, page 72]. The function R_α^H is an ordinary function or classical function if $\mathrm{Re}(\alpha) \geq n$ and is a distribution of α if $\mathrm{Re}(\alpha) < n$. Let $\operatorname{supp} R_\alpha^H(u) \subset \overline{\Gamma_+}$, where $\operatorname{supp} R_\alpha^H(u)$ denotes the support of $R_\alpha^H(u)$.

Definition 2.2. Let $x = (x_1, x_2, \dots, x_n)$ be a point of $\mathbb{R}^n$, and write $v = x_1^2 + x_2^2 + \cdots + x_n^2$. For any complex number β, define

$$R_\beta^e(v) = \frac{2^{-\beta}\pi^{-n/2}\Gamma((n-\beta)/2)\, v^{(\beta-n)/2}}{\Gamma(\beta/2)}. \tag{2.3}$$

The function $R_\beta^e(v)$ is called the elliptic kernel of Marcel Riesz and is an ordinary function for $\mathrm{Re}(\beta) \geq n$ and is a distribution of β for $\mathrm{Re}(\beta) < n$.

Definition 2.3. Let f be a continuous function, then the Fourier transform of f, denoted by $\mathfrak{J}f$ or $\hat{f}(\xi)$, is defined by

$$\mathfrak{J}f = \hat{f}(\xi) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-i(\xi,x)} f(x)\,dx, \tag{2.4}$$

where $x = (x_1, x_2, \dots, x_n) \in \mathbb{R}^n$, $\xi = (\xi_1, \xi_2, \dots, \xi_n) \in \mathbb{R}^n$, and $(\xi, x) = \xi_1 x_1 + \xi_2 x_2 + \cdots + \xi_n x_n$. From (2.4), the inverse Fourier transform of $\hat{f}(\xi)$ is defined by

$$f(x) = \mathfrak{J}^{-1}\hat{f}(\xi) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{i(\xi,x)} \hat{f}(\xi)\,dx. \tag{2.5}$$

If f is a distribution with compact support, by [8, Theorem 7.4.3, page 187] (2.5) can be written as

$$\mathfrak{J}f = \hat{f}(\xi) = \frac{1}{(2\pi)^{n/2}} \langle f(x), e^{-i(\xi,x)} \rangle. \tag{2.6}$$

Lemma 2.4. *Given the equation*

$$\diamond^k u(x) = \delta, \tag{2.7}$$

where $\diamond^k$ is the operator defined by (1.5), and δ is the Dirac-delta distribution, $u(x)$ is an unknown, k is a nonnegative integer and $x \in \mathbb{R}^n$, where n is odd with p odd, q even $(n = p + q)$. Then $u(x) = (-1)^k K_{2k,2k}(x)$ is an elementary solution of the operator $\diamond^k$. Here $K_{2k,2k}(x) = R_{2k}^H(u) * R_{2k}^e(v)$ from (1.4) with $\alpha = \beta = 2k$.

Proof. See [4, page 33]. □

In this paper, we study the spectrum of $(-1)^k K_{2k,2k}(x)$, relate to the residue of the Fourier transform $(-1)^k \widehat{K_{2k,2k}(\xi)}$.

Lemma 2.5. *The Fourier transform*

$$\begin{aligned} \widehat{K_{\alpha,\beta}(\xi)} &= (2\pi)^{n/2}\mathfrak{J}R_\alpha^H(u)\mathfrak{J}R_\beta^e(v) \\ &= \frac{(i)^q 2^{\alpha+\beta}\pi^n}{(2\pi)^{n/2}K_n(\alpha)H_n(\beta)} \cdot \frac{\Gamma(\alpha/2)\Gamma(\beta/2)}{\Gamma((n-\alpha)/2)\Gamma((n-\beta)/2)} \\ &\quad \times \left(\sqrt{\sum_{i=1}^{p}\xi_i^2 - \sum_{j=p+1}^{p+q}\xi_j^2}\right)^{-\alpha} \left(\sqrt{\sum_{i=1}^{n}\xi_i^2}\right)^{-\beta}, \quad i = \sqrt{-1}. \end{aligned} \tag{2.8}$$

In particular, if $\alpha = \beta = 2k$, k is a nonnegative integer,

$$(-1)^k \widehat{K_{2k,2k}(\xi)} = \frac{1}{(2\pi)^{n/2}} \frac{1}{\left((\xi_1^2 + \xi_2^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \xi_{p+2}^2 + \cdots + \xi_{p+q}^2)^2\right)^k}, \quad (2.9)$$

where $R_\alpha^H(u)$ and $R_\beta^\ell(v)$ are defined by (2.1) and (2.3), respectively.

Proof. See [2, page 194] and [5, pages 156–157]. □

Definition 2.6. The spectrum of the distributional kernel $K_{\alpha,\beta}(x)$ is the support of the Fourier transform $\widehat{K_{\alpha,\beta}(\xi)}$ or the spectrum of $K_{\alpha,\beta}(x) = \operatorname{supp}\widehat{K_{\alpha,\beta}(\xi)}$. Now, from Lemma 2.5 we obtain

$$\operatorname{supp}\widehat{K_{\alpha,\beta}(\xi)} = (\operatorname{supp}\mathfrak{J}R_\alpha^H(u)) \cap (\operatorname{supp}\mathfrak{J}R_\beta^\ell(v)). \quad (2.10)$$

In particular, from (2.9) the spectrum of

$$(-1)^k K_{2k,2k}(x) = \operatorname{supp}\left[\frac{1}{(2\pi)^{n/2}\left(\left(\sum_{i=1}^p \xi_i^2\right)^2 - \left(\sum_{j=p+1}^{p+q} \xi_j^2\right)^2\right)^k}\right]. \quad (2.11)$$

Lemma 2.7. *Let $P(x_1, x_2, \ldots, x_n)$ be a quadratic form of positive definite, and is defined by*

$$P = P(x_1, x_2, \ldots, x_n) = \left(\sum_{i=1}^p x_i^2\right)^2 - \left(\sum_{j=p+1}^{p+q} x_j^2\right)^2, \quad (2.12)$$

then for any testing function $\varphi(x) \in D$, the space of infinitely differentiable function with compact support,

$$\langle \delta^{(k)}(P), \varphi\rangle = \int_0^\infty \left[\left(\frac{\partial}{4s^3\partial s}\right)^k \left(s^{q-4}\frac{\psi(r,s)}{4}\right)\right]_{s=r} r^{p-1}\,dr, \quad (2.13)$$

$$\langle \delta^{(k)}(P), \varphi\rangle = (-1)^k \int_0^\infty \left[\left(\frac{\partial}{4r^3\partial r}\right)^k \left(r^{p-4}\frac{\psi(r,s)}{4}\right)\right]_{r=s} s^{q-1}\,ds, \quad (2.14)$$

where $r^2 = x_1^2 + x_2^2 + \cdots + x_p^2$, $s^2 = x_{p+1}^2 + x_{p+2}^2 + \cdots + x_{p+q}^2$, and

$$\psi(r,s) = \int \varphi\, d\Omega^p\, d\Omega^q, \quad (2.15)$$

where $d\Omega^p$ and $d\Omega^q$ are the elements of surface area on the unit sphere in $\mathbb{R}^p$ and $\mathbb{R}^q$, respectively. Both integrals (2.13) and (2.14) converge if $k < (1/4)(p+q-4)$ for any $\varphi(x) \in D$. If $k \geq (1/4)(p+q-4)$, these integrals must be understood in the sense of their regularization and (2.13) defined as $\langle \delta_1^{(k)}(p), \varphi\rangle$ and (2.14) defined as $\langle \delta_2^{(k)}(p), \varphi\rangle$. Moreover, if we put $u = r^2$, $v = s^2$, thus (2.13) and (2.14) become

$$\langle \delta^{(k)}(p), \varphi\rangle = \frac{1}{16}\int_0^\infty \left[\frac{\partial^k}{\partial v^k}\left(v^{(q-4)/4}\psi_1(u,v)\right)\right]_{v=u} u^{(1/4)(p-4)}\,du, \quad (2.16)$$

$$\langle \delta^{(k)}(p), \varphi\rangle = \frac{(-1)^k}{16}\int_0^\infty \left[\frac{\partial^k}{\partial u^k}\left(u^{(p-4)/4}\psi_1(u,v)\right)\right]_{u=v} v^{(1/4)(q-4)}\,dv, \quad (2.17)$$

where $\psi_1(u,v) = \psi(r,s)$.

Proof. See [2, pages 247–251]. □

Lemma 2.8. *Let $G_b = \{\xi \in \mathbb{R}^n : |\xi_1| \le b_1, |\xi_2| \le b_2, \dots, |\xi_n| \le b_n\}$ be a parallelepiped in $\mathbb{R}^n$ and b_i $(1 \le i \le n)$ is a real constant and the inverse Fourier transform of $\widehat{K_{\alpha,\beta}(\xi)}$ is defined by*

$$K_{\alpha,\beta}(x) = \mathfrak{I}^{-1}\widehat{K_{\alpha,\beta}(\xi)} = \frac{1}{(2\pi)^{n/2}} \int_{G_b} e^{i(\xi,x)} \widehat{K_{\alpha,\beta}(\xi)}\, d\xi, \tag{2.18}$$

where $K_{\alpha,\beta}$ is defined by (1.4) and $x, \xi \in \mathbb{R}^n$, then $K_{\alpha,\beta}(x)$ can be extended to the entire function $K_{\alpha,\beta}(z)$ and be analytic for all $z = (z_1, z_2, \dots, z_n) \in \mathbb{C}^n$, where $\mathbb{C}^n$ is the n-tuple space of complex number and

$$|K_{\alpha,\beta}(z)| \le C \exp(b|\operatorname{Im}(z)|), \tag{2.19}$$

where $\exp(b|\operatorname{Im}(z)|) = \exp[b_1|\operatorname{Im}(z_1)| + b_2|\operatorname{Im}(z_2)| + \cdots + b_n|\operatorname{Im}(z_n)|]$ and $C = (1/(2\pi)^{n/2}) \int_{G_b} |\widehat{K_{\alpha,\beta}(\xi)}| d\xi$ is a constant. Moreover, $K_{\alpha,\beta}(x)$ has a spectrum contained in G_b.

Proof. Since the integral of (2.18) converges for all $\xi \in G_b$, thus $K_{\alpha,\beta}(x)$ can be extended to the entire function $K_{\alpha,\beta}(z)$ and be analytic for all $z \in C^n$. Thus (2.18) can be written as

$$K_{\alpha,\beta}(z) = \frac{1}{(2\pi)^{n/2}} \int_{G_b} e^{i(\xi,z)} \widehat{K_{\alpha,\beta}(\xi)}\, d\xi. \tag{2.20}$$

Now,

$$\begin{aligned} |K_{\alpha,\beta}(z)| &\le \frac{1}{(2\pi)^{n/2}} \int_{G_b} |\widehat{K_{\alpha,\beta}(\xi)}|\, |\exp(i\xi_1 z_1 + i\xi_2 z_2 + \cdots + i\xi_n z_n)|\, d\xi \\ &= \frac{1}{(2\pi)^{n/2}} \int_{G_b} |\widehat{K_{\alpha,\beta}(\xi)}|\, |\exp(i\xi_1\sigma_1 + i\xi_2\sigma_2 + \cdots + i\xi_n\sigma_n \\ &\qquad - \xi_1\mu_1 - \xi_2\mu_2 - \cdots - \xi_n\mu_n)|\, d\xi, \end{aligned} \tag{2.21}$$

where

$$z_j = \sigma + i\mu_j \quad (j = 1, 2, \dots, n), \tag{2.22}$$

thus

$$|K_{\alpha,\beta}(z)| \le \frac{1}{(2\pi)^{n/2}} \int_{G_b} |\widehat{K_{\alpha,\beta}(\xi)}|\, d\xi \exp(b_1|\mu_1| + b_2|\mu_2| + \cdots + b_n|\mu_n|) \tag{2.23}$$

for $|\xi_j| \le b_j$, or $|K_{\alpha,\beta}(z)| \le C\exp(b_1|\operatorname{Im}(z_1)| + b_2|\operatorname{Im}(z_2)| + \cdots + b_n|\operatorname{Im}(z_n)|)$, or $|K_{\alpha,\beta}(z)| \le C\exp(b|\operatorname{Im}(z)|)$, where $C = (1/(2\pi)^{n/2}) \int_{G_b} |\widehat{K_{\alpha,\beta}(\xi)}| d\xi$ is a constant. □

We must show that the support of $\widehat{K_{\alpha,\beta}(\xi)}$ is contained in G_b. Since $K_{\alpha,\beta}(z)$ is an analytic function that satisfies the inequality (2.19) and is called an entire function of order of growth ≤ 1 and of type $\le b$, then by Paley-Wiener-Schartz theorem, see [3, page 162], $\widehat{K_{\alpha,\beta}(\xi)}$ has a support contained in G_b, that is the spectrum of $K_{\alpha,\beta}(x)$ is contained in G_b.

In particular, for $\alpha = \beta = 2k$, the spectrum of $(-1)^k K_{2k,2k}(x)$ is also contained in G_b, that is $\operatorname{supp}[(-1)^k \widehat{K_{2k,2k}(\xi)}] \subset G_b$, where $(-1)^k K_{2k,2k}(x)$ is an elementary solution of the Diamond operator $\diamond^k$ by Lemma 2.4, and the Fourier transform $(-1)^k \widehat{K_{2k,2k}(\xi)}$ given by (2.9) can be defined as follows.

Definition 2.9. The Fourier transform

$$(-1)^k \widehat{K_{2k,2k}(\xi)} = \begin{cases} \dfrac{1}{(2\pi)^{n/2}\left[\left(\sum_{i=1}^{p}\xi_i^2\right)^2 - \left(\sum_{j=p+1}^{p+q}\xi_j^2\right)^2\right]^k}, & \text{for } \xi \in G_b, \\ 0, & \text{for } \xi \in CG_b, \end{cases} \tag{2.24}$$

where $\xi = (\xi_1, \xi_2, \dots, \xi_n) \in \mathbb{R}^n$ and CG_b is the complement of G_b.

3. Main results

Theorem 3.1. *For any nonzero point $\xi \in M$ where M is a spectrum of $(-1)^k K_{2k,2k}(x)$, and $(-1)^k K_{2k,2k}(x)$ is an elementary solution of the operator $\diamond^k$ by Lemma 2.4. Then there exists the residue of the Fourier transform $(-1)^k \widehat{K_{2k,2k}(\xi)}$ at the singular point $\lambda = -k$ and such a residue is*

$$\frac{(-1)^{k-1}}{(2\pi)^{n/2}(k-1)!}\delta_1^{(k-1)(p)} \quad \text{or} \quad \operatorname{res}_{\lambda=-k}(-1)^k \widehat{K_{2k,2k}(\xi)} = \frac{(-1)^{k-1}}{(2\pi)^{n/2}(k-1)!}\delta^{(k-1)(p)}, \tag{3.1}$$

where

$$P = (\xi_1^2 + \xi_2^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \xi_{p+2}^2 + \cdots + \xi_{p+q}^2), \tag{3.2}$$

$p + q = n$ and $\delta_1^{(k-1)}(P)$ is defined by (2.16) with $\delta^{(k-1)}(P) = \delta_1^{(k-1)}(P)$ and n is odd with p odd, q even.

Proof. We define the generalized function P^λ, where P is given by (3.2) and λ is a complex number, by

$$\langle P^\lambda, \varphi \rangle = \int_{P>0} P^\lambda(\xi)\varphi(\xi)\,d\xi, \tag{3.3}$$

where $\xi = (\xi_1, \xi_2, \dots, \xi_n)$ and $d\xi = d\xi_1 d\xi_2 \cdots d\xi_n$ and $\varphi(\xi) \in D$, the space of continuous infinitely differentiable function with compact support. Now,

$$\langle P^\lambda, \varphi \rangle = \int_{P>0} \left[(\xi_1^2 + \xi_2^2 + \cdots + \xi_p^2)^2 - (\xi_{p+1}^2 + \xi_{p+2}^2 + \cdots + \xi_{p+q}^2)\right]^\lambda \varphi(\xi)\,d\xi. \tag{3.4}$$

We transform to bipolar coordinates defined by

$$\begin{gathered} \xi_1 = rw_1,\ \xi_2 = rw_2,\ \dots,\ \xi_p = rw_p, \\ \xi_{p+1} = sw_{p+1},\ \xi_{p+2} = sw_{p+2},\ \dots,\ \xi_{p+q} = sw_{p+q}, \quad p+q = n, \end{gathered} \tag{3.5}$$

where $\sum_{i=1}^{p} w_i^2 = 1$ and $\sum_{j=p+1}^{p+q} w_j^2 = 1$. Thus

$$r = \sqrt{\sum_{i=1}^{p}\xi_i^2}, \qquad s = \sqrt{\sum_{j=p+1}^{p+q}\xi_j^2}. \tag{3.6}$$

We have $\langle P^\lambda, \varphi\rangle = \int [r^4 - s^4]^\lambda \varphi(\xi) d\xi$. Since the volume $d\xi = r^{p-1}s^{q-1}\,dr\,ds\,d\Omega_p\,d\Omega_q$ where $d\Omega_p$ and $d\Omega_q$ are the elements of surface area on the unit sphere in $\mathbb{R}^p$ and $\mathbb{R}^q$, respectively. Thus

$$\begin{aligned}\langle P^\lambda, \varphi\rangle &= \int_{p>0} (r^4 - s^4)^\lambda \varphi r^{p-1} s^{q-1}\,dr\,ds\,d\Omega^p\,d\Omega^q \\ &= \int_0^\infty \int_0^r (r^4 - s^4)^\lambda \psi(r,s) r^{p-1} s^{q-1}\,ds\,dr,\end{aligned} \tag{3.7}$$

where $\psi(r,s) = \int \varphi\,d\Omega_p\,d\Omega_q$.

Since $\varphi(\xi)$ is in D, then $\psi(r,s)$ is an infinitely differentiable function of r^4 and s^4 with bounded support. We now make the change of variable $u = r^4$, $v = s^4$, and writing $\psi(r,s) = \psi_1(u,v)$. Thus we obtain

$$\langle P^\lambda, \varphi\rangle = \frac{1}{16}\int_{u=0}^\infty \int_{v=0}^u (u-v)^\lambda \psi_1(u,v) u^{(p-4)/4} v^{(q-4)/4}\,dv\,du. \tag{3.8}$$

Write $v = ut$. We obtain

$$\langle P^\lambda, \varphi\rangle = \frac{1}{16}\int_0^\infty u^{\lambda+(1/4)(p+q)-1}\,du \int_0^1 (1-t)^\lambda t^{(q-4)/4} \psi_1(u,ut)\,dt. \tag{3.9}$$

Let the function

$$\Phi(\lambda,u) = \frac{1}{16}\int_0^1 (1-t)^\lambda t^{(q-4)/4}\psi_1(u,ut)\,dt. \tag{3.10}$$

Thus $\Phi(\lambda,u)$ has singularity at $\lambda = -k$ where it has simple poles. By Gel'fand and Shilov [2, page 254, equation (12)] we obtain the residue of $\Phi(\lambda,u)$ at $\lambda = -k$, that is,

$$\operatorname{res}_{\lambda=-k}\Phi(\lambda,u) = \frac{1}{16}\frac{(-1)^{k-1}}{(k-1)!}\left[\frac{\partial^{k-1}}{\partial t^{k-1}}\{t^{(q-4)/4}\psi_1(u,ut)\}\right]_{t=1}. \tag{3.11}$$

Thus, $\operatorname{res}_{\lambda=-k}\Phi(\lambda,u)$ is a functional concentrated on the surface $P = 0$ ($t = 1$, $u = v$, $p = u - v = 0$). On the other hand, from (3.9) and (3.10) we have

$$\langle P^\lambda, \varphi\rangle = \int_0^\infty u^{\lambda+(1/4)(p+q)-1}\Phi(\lambda,u)\,du. \tag{3.12}$$

Thus $\langle P^\lambda, \varphi\rangle$ in (3.12) has singularities at $\lambda = -n/4, -n/4-1, \ldots, -n/4-k$. At these points,

$$\operatorname{res}_{\lambda=-n/4-k}\langle P^\lambda, \varphi\rangle = \frac{1}{k!}\left[\frac{\partial^k}{\partial u^k}\Phi\left(-\frac{n}{4}-k,u\right)\right]_{u=0}. \tag{3.13}$$

Thus the residue of $\langle P^\lambda, \varphi\rangle$ at $\lambda = (-1/2)n - k$ is a functional concentrated on the vertex of the surface P. Now consider the case when the singular point $\lambda = -k$. Write (3.10) in the neighborhood of $\lambda = -k$ in the form $\Phi(\lambda,u) = \Phi_0(u)/(\lambda+k) + \Phi_1(\lambda,u)$ where $\Phi_0(u) = \operatorname{res}_{\lambda=-k}\Phi(\lambda,u)$ and $\Phi_1(\lambda,u)$ is regular at $\lambda = -k$. Substitute $\Phi(\lambda,u)$ into (3.12) we obtain

$$\langle P^\lambda, \varphi\rangle = \frac{1}{\lambda+k}\int_0^\infty u^{\lambda+(1/4)(p+q)-1}\Phi_0(u)\,du + \int_0^\infty u^{\lambda+(1/4)(p+q)-1}\Phi_1(\lambda,u)\,du. \tag{3.14}$$

Thus $\operatorname{res}_{\lambda=-k}\langle P^{\lambda},\varphi\rangle = \int_0^{\infty} u^{-k+(1/4)(p+q)-1}\Phi_0(u)\,du$. By substituting $\Phi_0(u)$ and (3.11), we obtain .

$$\operatorname{res}_{\lambda=-k}\langle P^{\lambda},\varphi\rangle = \frac{(-1)^k}{16(k-1)!}\int_0^{\infty}\left[\frac{\partial^{k-1}}{\partial t^{k-1}}\{t^{1(q-4)/4}\psi_1(u,ut)\}\right]_{t=1} u^{-k+(1/4)(p+q)-1}\,du \tag{3.15}$$

since, we put $v = ut$. Thus $\partial^{k-1}/\partial t^{k-1} = u^{k-1}(\partial^{k-1}/\partial v^{k-1})$, by substituting $\partial^{k-1}/\partial t^{k-1}$ we obtain

$$\operatorname{res}_{\lambda=-k}\langle P^{\lambda},\varphi\rangle = \frac{(-1)^k}{16(k-1)!}\int_0^{\infty}\left[\frac{\partial^{k-1}}{\partial t^{k-1}}\{v^{1(q-4)/4}\psi_1(u,v)\}\right]_{u=v} u^{(1/4)p-1}\,du. \tag{3.16}$$

Now, by (2.16)

$$\operatorname{res}_{\lambda=-k}\langle P^{\lambda},\varphi\rangle = \frac{(-1)^{k-1}}{(k-1)!}\delta_1^{(k-1)}(P). \tag{3.17}$$

Since, by Definition 2.9 we have

$$(-1)^k\widehat{K_{2k,2k}(\xi)} = \frac{1}{(2\pi)^{n/2}}P^{\lambda} \quad \text{for } \lambda = -k, \tag{3.18}$$

and $\xi \in G_b$. Let M be a spectrum of $(-1)^k K_{2k,2k}(x)$ and $M \subset G_b$ by Lemma 2.8. Thus for any nonzero $\xi \in M$ we can find the residue of $(-1)^k\widehat{K_{2k,2k}(\xi)}$, that is,

$$\begin{aligned}\operatorname{res}_{\lambda=-k}\langle(-1)^k\widehat{K_{2k,2k}(\xi)},\varphi(\xi)\rangle &= \frac{1}{(2\pi)^{n/2}}\operatorname{res}_{\lambda=-k}\langle P^{\lambda},\varphi\rangle \\ &= \frac{(-1)^{k-1}}{(2\pi)^{n/2}(k-1)!}\langle\delta_1^{(k-1)}(P),\varphi\rangle\end{aligned} \tag{3.19}$$

or $\operatorname{res}_{\lambda=-k}(-1)^k\widehat{K_{2k,2k}(\xi)} = ((-1)^{k-1}/(2(\pi)^{n/2}(k-1)!))\delta_1^{(k-1)}(P)$ for $\xi \in M$ and $\xi \neq 0$.

Now consider the case $\xi = 0$. We have from (3.13) that, the residue of $\langle P^{\lambda},\varphi\rangle$ occurs at the point $\lambda = (-1/2)n-k$ that is $\operatorname{res}_{\lambda=-(1/2)n-k}\langle P^{\lambda},\varphi\rangle$ is a functional concentrated on the vertex of surface P. Since $u = 0$ and $v = ut$, then $u = v = 0$, that implies

$$\sqrt{\xi_1^2+\xi_2^2+\cdots+\xi_p^2} = \sqrt{\xi_{p+1}^2+\xi_{p+2}^2+\cdots+\xi_{p+q}^2} = 0. \tag{3.20}$$

It follows that $\xi_1 = \xi_2 = \cdots = \xi_{p+q} = 0$, $p+q = n$. Thus, the residue of $\langle P^{\lambda},\varphi\rangle$ is concentrated on the point $\xi = 0$.

Since, from Definition 2.9, $(1/(2\pi)^{n/2})P^{\lambda} = (-1)^k\widehat{K_{2k,2k}(\xi)}$ if $\lambda = -k$. Thus we only consider the residue of $(-1)^k\widehat{K_{2k,2k}(\xi)}$ at $\lambda = -k$. From (3.12), we consider the residue of $\langle P^{\lambda},\varphi\rangle$ only at $\lambda = -k$. That implies $(1/4)(p+q)-1 = 0$ or $n = 4$ $(p+q = n)$. Since $n = 4$ is an even dimension which contradicts Lemma 2.4, the existence of the elementary solution $(-1)^k K_{2k,2k}(x)$ that exists for odd n. Thus cases (3.12) and (3.13) do not occur. This implies that the case $\xi = 0$ does not happen. It follows that

$$\operatorname{res}_{\lambda=-k}(-1)^k\widehat{K_{2k,2k}(\xi)} = \frac{(-1)^{k-1}}{(2\pi)^{n/2}(k-1)!}\delta_1^{(k-1)}(P) \tag{3.21}$$

for nonzero point $\xi \in M$ concentrated on the surface $P = 0$, where M is a spectrum of $(-1)^k K_{2k,2k}(x)$. □

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On the Diamond Operator related to the Wave Equation

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Abstract

In this paper, we study the solution of the equation $\diamondsuit^k u(x) = f(x)$ where $\diamondsuit^k$ is the Diamond operator iterated k times and is defined by

$$\diamondsuit^k = \left(\left(\sum_{i=1}^{p} \frac{\partial^2}{\partial x_i^2}\right)^2 - \left(\sum_{j=p+1}^{p+q} \frac{\partial^2}{\partial x_j^2}\right)^2\right)^k$$

where $p+q=n$ is the dimension of the n-dimensional Euclidean space $R^n, x = (x_1, x_2, ..., x_n) \in R^n, k$ is a nonnegative integer, $u(x)$ is an unknown and f is a generalized function.

It is found that the solution $u(x)$ depends on the conditions of p and q and moreover such a solution is related to the solution of the Laplace equation and the wave equation.

1 Introduction

The operator $\diamondsuit^k$ has been first introduced by A. Kananthai [3] and is named as the Diamond operater iterated k times and is defined by

$$\begin{aligned} \diamondsuit^k \;=\; & ((\tfrac{\partial^2}{\partial x_1^2} + \tfrac{\partial^2}{\partial x_2^2} + \cdots + \tfrac{\partial^2}{\partial x_p^2})^2 - \\ & (\tfrac{\partial^2}{\partial x_{p+1}^2} + \tfrac{\partial^2}{\partial x_{p+2}^2} + \cdots + \tfrac{\partial^2}{\partial x_{p+q}^2})^2)^k \end{aligned} \tag{1.1}$$

where $p+q=n$ is the dimension of the space $R^n, x = (x_1, x_2, ..., x_n) \in R^n$ and k is a nonnegative integer.

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Actually the operator $\diamondsuit^k$ is an extension of the ultrahyperbolic operator and the Laplacian. So the operator $\diamondsuit^k$ can be expressed as the product of the operator $\Box$ and $\triangle$, that is $\diamondsuit^k = \Box^k\triangle^k = \triangle^k\Box^k$ where

$$\Box^k = \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \cdots + \frac{\partial^2}{\partial_p^2} - \frac{\partial^2}{\partial x_{p+1}^2} - \frac{\partial^2}{\partial x_{p+2}^2} - \cdots - \frac{\partial^2}{\partial x_{p+q}^2}\right)^k \quad (1.2)$$

is the ultrahyperbolic operator iterated k-time with $p + q = n$, and

$$\triangle^k = \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \cdots + \frac{\partial^2}{\partial x_n^2}\right)^k \quad (1.3)$$

is the Laplacian iterated k-times.

A. Kananthai ([3], Theorem 3.1 p33) has shown that the convolution $(-1)^k R^e_{2k}(x) * R^H_{2k}(x)$ is an elementory solution of the operator $\diamondsuit^k$, that is

$$\diamondsuit^k \left((-1)^k R^e_{2k}(x) * R^H_{2k}(x)\right) = \delta \quad (1.4)$$

where δ is the Dirac-delta distribution and the functions R^e_{2k} and R^H_{2k} are defined by (2.5) and (2.1) respectively with $\alpha = 2k, k$ is nonnegative integer.

In this paper, we study the solution of the equation

$$\diamondsuit^k u(x) = f(x) \quad (1.5)$$

This equation is the geheralization of the ultrahyperbolic equation and it can be applied to the wave equation and potential that has been shown in the last part of this paper.

Let $K_{\alpha,\beta}(x)$ be a distributional family and is defined by

$$K_{\alpha,\beta}(x) = R^e_\alpha * R^H_\beta \quad (1.6)$$

where R^e_α is called the elliptic Kernel defined by (2.5) and R^H_β is called the ultra-hyperbolic Kernel defined by (2.1) and α, β are the complex parameters.

The family $K_{\alpha,\beta}(x)$ is well-defined and is a tempered distribution, since $R^e_\alpha * R^H_\beta$ is a tempered, see ([1], Lemma 2.2) and R^H_β has a compact support.

In this paper, we can show that

$$u(x) = (-1)^k R^e_{2k}(x) * \left(R^H_{2(k-1)}(v)\right)^{(m)} + (-1)^k K_{2k,2k}(x) * f(x)$$

is a solution of (1.5) where m $= \frac{n-4}{2}, n \geq 4$ and n is even number and $k_{2k,2k}(x)$ is defined by (1.6) with $\alpha = \beta = 2k$. Moreover, we can show that the solution u(x) relates to the solution of Laplace operator $\triangle^{2k}$ defined by (1.3)and also the wave operator defined by (1.2) with $k = 1$ and $p = 1$.

2 Preliminaries

Definition 2.1 Let $x = (x_1, x_2, ..., x_n)$ be a point of the n-dimensional Euclidean space R^n.

Denote by $v = x_1^2 + x_2^2 + \cdots + x_p^2 - x_{p+1}^2 - x_{p+2}^2 - \cdots - x_{p+q}^2, p + q = n$ the nondegenerated quadratic form. By Γ_+ we designate the interior of the forward cone.

$\Gamma_+ = \{x \in R^n : x_1 > 0\, and\, v > 0\}$, and by $\overline{\Gamma}_+$ designate its closure. For any complex number α, define

$$R_\alpha^H(v) = \begin{cases} \frac{v^{(\alpha-n)/2}}{K_n(\alpha)} & \text{for } x \in \Gamma_+ \\ 0 & \text{for } x \notin \Gamma_+ \end{cases} \tag{2.1}$$

where $K_n(\alpha)$ is given by the formula

$$K_n(\alpha) = \frac{\pi^{(n-1)/2}\Gamma\left(\frac{2+\alpha-n}{2}\right)\Gamma\left(\frac{1-\alpha}{2}\right)\Gamma(\alpha)}{\Gamma\left(\frac{2+\alpha-p}{2}\right)\Gamma\left(\frac{p-\alpha}{2}\right)}. \tag{2.2}$$

The function $R_\alpha^H(x)$ was introduced by Nozaki ([4], p.72).

It is well known that $R_\alpha^H(x)$ is an ordinary function if $Re(\alpha) \geq n$ and it is a distribution of α if $Re(\alpha) < n$. Let supp$R_\alpha^H(x)$ denote the support of $R_\alpha^H(x)$. Suppose that supp$R_\alpha^H(x) \subset \overline{\Gamma}_+$.

From S.E Trione ([5], p11), $R_{2k}^H(v)$ is an elementary solution of the operator $\Box^k$ that is

$$\Box^k R_{2k}^H(v) = \delta \tag{2.3}$$

where $\Box^k$ is defined by (1.2).

By putting $p = 1$ in (2.1) and (2.2) and remembering the Legendre's duplication of $\Gamma(z)$.

$\Gamma(2z) = 2^{2z-1}\pi^{-1/2}\Gamma(z)\Gamma\left(z + \frac{1}{2}\right)$ then the formula (2.1) reduces to

$$M_\alpha(v) = \begin{cases} \frac{v^{(\alpha-n)/2}}{H_n(\alpha)} & \text{if } x \in \Gamma_+ \\ 0 & \text{if } x \notin \Gamma_+ \end{cases} \tag{2.4}$$

Here $v = x_1^2 - x_2^2 - \cdots - x_n^2$ and $H_n(\alpha) = \pi^{(n-2)/2}2^{\alpha-1}\Gamma\left(\frac{\alpha-n+2}{2}\right)\Gamma\left(\frac{\alpha}{2}\right)$.

$M_\alpha(v)$ is, precisely, the hyperbolic kernel of Marcel Riesz.

Definition 2.2 Let $x = (x_1, x_2, ..., x_n)$ be a point of R^n and the function $R_\alpha^e(x)$ be defined by

$$R_\alpha^e(x) = \frac{|x|^{\alpha-n}}{W_n(\alpha)} \tag{2.5}$$

where $W_n(\alpha) = \frac{\pi^{n/2}2^\alpha\Gamma(\frac{\alpha}{2})}{\Gamma(\frac{n-\alpha}{2})}$, α is a complex parameter and $|x| = (x_1^2 + x + 2^2 + \cdots + x_n^2)^{1/2}$.

It can be shown that $R_{-2k}^e(x) = (-1)^k\Delta^k\delta(x)$ where Δ^k is defined by (1.3). It follows that $R_0^e(x) = \delta$, see ([2], p118).

Moreover, we obtain $(-1)^k R^e_{2k}(x)$ is an elementary solution of the operator $\triangle^k$, that is

$$\triangle^k \left((-1)^k R^e_{2k}(x)\right) = \delta \tag{2.6}$$

see ([3] , Lemma 2.4 p31).

Lemma 2.1 Given P is a hyper-surface then

$$P\delta^{(k)}(P) + k\delta^{(k-1)}(P) = 0$$

where $\delta^{(k)}$ is the Dirac-delta distribution with k derivatives.
Proof. See ([1], P233).

Lemma 2.2 Given the equation

$$\triangle^k u(x) = 0 \tag{2.7}$$

where $\triangle^k$ is defined by (1.3) and $x = (x_1, x_2, ..., x_n) \in R^n$ then $u(x) = (-1)^{(k-1)} \left(R^e_{2(k-1)}(x)\right)^{(m)}$ is a solution of (2.7) where m is a nonnegative integer with $m = \frac{n-4}{2}, n \geq 4$ and n is even and $\left(R^e_{2(k-1)}(x)\right)^{(m)}$ is a function defined by (2.5) with m derivatives with $\alpha = 2(k-1)$
Proof. We first show that the generalized function $u(x) = \delta^{(m)}(r^2)$ where $r^2 = |x|^2 = x_1^2 + x_2^2 + \cdots + x_n^2$ is a solution of

$$\triangle u(x) = 0 \tag{2.8}$$

where $\triangle = \sum_{i=1}^n \frac{\partial^2}{\partial x_i^2}$ is a Laplace operator.Now

$$\begin{aligned} \frac{\partial}{\partial x_i}\delta^{(m)}(r^2) &= 2x_i\delta^{(m+1)}(r^2) \\ \frac{\partial^2}{\partial x_i^2}\delta^{(m)}(r^2) &= 2\delta^{(m+1)}(r^2) + 4x_i^2\delta^{(m+2)}(r^2). \end{aligned}$$

Thus

$$\begin{aligned} \triangle\delta^{(m)}(r^2) &= \sum_{i=1}^n \frac{\partial^2}{\partial x_i^2}\delta^{(m)}(r^2) \\ &= 2n\delta^{(m+1)}(r^2) + 4r^2\delta^{(m+2)}(r^2) \\ &= 2n\delta^{(m+1)}(r^2) - 4(m+2)\delta^{(m+1)}(r^2) \end{aligned}$$

by Lemma 2.1 with $P = r^2$.We have

$$\begin{aligned} \triangle\delta^{(m)}(r^2) &= [2n - 4(m+2)]\delta^{(m+1)}(r^2) \\ &= 0 \quad \text{if } 2n - 4(m+2) = 0 \end{aligned}$$

or $m = \frac{n-4}{2}, n \geq 4$ and n is even. Thus $\delta^{(m)}(r^2)$ is a solution of (2.8) with $m = \frac{n-4}{2}, n \geq 4$ and n is even. Now $\triangle^k u(x) = \triangle(\triangle^{k-1}u(x)) = 0$ then from the above proof $\triangle^{k-1}u(x) = \delta^{(m)}(r^2)$ with $m = \frac{n-4}{2}, n \geq 4$ and n is even.

Convolving both sides of the above equation by the function $(-1)^{k-1}R^e_{2(k-1)}(x)$, we obtain

$$\begin{aligned}(-1)^{k-1}R^e_{2(k-1)}(x) * \triangle^{k-1}u(x) &= (-1)^{k-1}R^e_{2(k-1)}(x) * \delta^{(m)}(r^2)\\ \text{or } \triangle^{k-1}\left((-1)^{k-1}R^e_{2(k-1)}(x)\right) * u(x) &= (-1)^{k-1}R^e_{2(k-1)}(x) * \delta^{(m)}(r^2)\end{aligned}$$

$$\text{or} \qquad \delta * u(x) = u(x) = (-1)^{k-1}R^e_{2(k-1)}(x) * \delta^{(m)}(r^2) \quad \text{by (2.6)}$$

Now from (2.1)

$$\begin{aligned}R^e_{2(k-1)}(x) &= \frac{|x|^{2(k-1)-n}}{W_n(\alpha)}\\ &= \frac{\left(|x|^2\right)^{\frac{2(k-1)-n}{2}}}{W_n(\alpha)} = \frac{\left(r^2\right)^{\frac{2(k-1)-n}{2}}}{W_n(\alpha)}\end{aligned}$$

where $r = |x| = (x_1^2 + x_2^2 + \cdots + x_n^2)^{1/2}$. Hence

$$\begin{aligned}R^e_{2(k-1)}(x) * \delta^{(m)}(r^2) &= \frac{\left(r^2\right)^{\frac{2(k-1)-n}{2}}}{W_n(\alpha)} * \delta^{(m)}(r^2)\\ &= \left[\frac{\left(r^2\right)^{\frac{2(k-1)-n}{2}}}{W_n(\alpha)}\right]^{(m)} = \left[R^e_{2(k-1)}(x)\right]^{(m)}.\end{aligned}$$

It follows that $u(x) = (-1)^{k-1}\left[R^e_{2(k-1)}(x)\right]^{(m)}$ is a solution of (2.7) with $m = \frac{n-4}{2}, n \geq 4$ and n is even dimension of R^n.

Lemma 2.3 Given the equation

$$\Box^k u(x) = 0 \tag{2.9}$$

where $\Box^k$ is defined by (1.2) and $x = (x_1, x_2, ..., x_n) \in R^n$ then $u(x) = \left[R^H_{2(k-1)}(v)\right]^{(m)}$ is a solution of (2.9) with $m = \frac{n-4}{n}, n \geq 4$ and n is even dimension and v is defined by Definition 2.1. The function $\left[R^H_{2(k-1)}(v)\right]^{(m)}$ is defined by (2.1) with m-derivatives and $\alpha = 2(k-1)$.

Proof At first we show that the generalized function $\delta^{(m)}(r^2 - s^2)$ where $r^2 = x_1^2 + x_2^2 + \cdots + x_p^2$ and $s^2 = x_{p+1}^2 + x_{p+2}^2 + \cdots + x_{p+q}^2, p + q = n$, is a solution of the equation

$$\Box u(x) = 0 \tag{2.10}$$

where $\Box$ is defined by (1.2) with $k = 1$ and $x = (x_1, x_2, ..., x_n) \in R^n$. Now

$$\begin{aligned}
\frac{\partial}{\partial x_i}\delta^{(m)}(r^2-s^2) &= 2x_i\delta^{(m+1)}(r^2-s^2)\\
\frac{\partial^2}{\partial x_i^2}\delta^{(m)}(r^2-s^2) &= 2\delta^{(m+1)}(r^2-s^2)+4x_i^2\delta^{(m+2)}(r^2-s^2)\\
\sum_{i=1}^{p}\frac{\partial^2}{\partial x_i^2}\delta^{(m)}(r^2-s^2) &= 2p\delta^{(m+1)}(r^2-s^2)+4r^2\delta^{(m+2)}(r^2-s^2)\\
&= 2p\delta^{(m+1)}(r^2-s^2)\\
&\quad +4(r^2-s^2)\delta^{(m+2)}(r^2-s^2)\\
&\quad +4s^2\delta^{(m+2)}(r^2-s^2)\\
&= 2p\delta^{(m+1)}(r^2-s^2)\\
&\quad -4(m+2)\delta^{(m+1)}(r^2-s^2)\\
&\quad +4s^2\delta^{(m+2)}(r^2-s^2)\\
&= [2p-4(m+2)]\delta^{(m+1)}(r^2-s^2)\\
&\quad +4s^2\delta^{(m+2)}(r^2-s^2)
\end{aligned}$$

by Lemma 2.1 with $P=r^2-s^2$.
Similarly,

$$\begin{aligned}
\sum_{j=p+1}^{p+q}\frac{\partial^2}{\partial x_j^2}\delta^{(m)}(r^2-s^2) &= [-2q+4(m+2)]\delta^{(m+1)}(r^2-s^2)\\
&\quad +4r^2\delta^{(m+2)}(r^2-s^2).
\end{aligned}$$

Thus

$$\begin{aligned}
\Box\delta^{(m)}(r^2-s^2) &= \sum_{i=1}^{p}\frac{\partial^2}{\partial x_i^2}\delta^{(m)}(r^2-s^2)-\sum_{j=p+1}^{p+q}\frac{\partial^2}{\partial x_j^2}\delta^{(m)}(r^2-s^2)\\
&= [2(p+q)-8(m+2)]\delta^{(m+1)}(r^2-s^2)\\
&\quad -4(r^2-s^2)\delta^{(m+2)}(r^2-s^2)\\
&= [2n-8(m+2)]\delta^{(m+1)}(r^2-s^2)\\
&\quad +4(m+2)\delta^{(m+1)}(r^2-s^2) \quad \text{by Lemma 2.1}\\
&= [2n-4(m+2)]\delta^{(m+1)}(r^2-s^2).
\end{aligned}$$

If $2n-4(m+2)=0$, we have $\Box\delta^{(m)}(r^2-s^2)=0$. That is $u(x)=\delta^{(m)}(r^2-s^2)$ is a solution of (2.10) with $m=\frac{n-4}{2}, n\geq 4$ and n is even dimension. Now $\Box^k u(x)=\Box\left(\Box^{k-1}u(x)\right)=0$.

From (2.10) we have $\Box^{k-1}u(x)=\delta^{(m)}(r^2-s^2)$ with $m=\frac{n-4}{2}, n\geq 4$ and n is even dimension.

Convolving the above equation by $R^H_{2(k-1)}(v)$, we obtain

$$\begin{aligned}
R^H_{2(k-1)}(v)*\Box^{k-1}u(x) &= R^H_{2(k-1)}(v)*\delta^{(m)}(r^2-s^2)\\
\Box^{k-1}\left[R^H_{2(k-1)}(v)\right]*u(x) &= \left[R^H_{2(k-1)}(v)\right]^{(m)} \text{ where } v=r^2-s^2\\
\delta*u(x)=u(x) &= \left[R^H_{2(k-1)}(v)\right]^{(m)}
\end{aligned}$$

by (2.3) and $v=r^2-s^2$ is defined by Definition 2.1.

Thus $u(x)=\left[R^H_{2(k-1)}(v)\right]^{(m)}$ is a solution of (2.9) with $m=\frac{n-4}{2}, n\geq 4$ and n is even dimension.

Lemma 2.4 Given the equation

$$\diamondsuit^k u(x) = 0 \tag{2.11}$$

where $\diamondsuit^k$ is the Diamond operator iterated k-times defined by (1.1) and $u(x)$ is an unknown generalized function.Then

$$u(x) = (-1)^k R^e_{2k}(x) * \left(R^H_{2(k-1)}(v)\right)^{(m)} \tag{2.12}$$

is a solution of (2.11), $\left(R^H_{2(k-1)}(v)\right)^{(m)}$ is a function with m-derivatives defined by (2.1) and v is defined by definition 2.1.

Proof Now $\diamondsuit^k u(x) = \Box^k \Delta^k u(x) = 0$. By Lemma 2.3 ,$\Delta^k u(x) = \left(R^H_{2(k-1)}(v)\right)^{(m)}$.

Convolving both sides by $(-1)^k R^e_{2k}(x)$, we have

$$(-1)^k R^e_{2k}(x) * \Delta^k u(x) = (-1)^k R^e_{2k}(x) * \left(R^H_{2(k-1)}(v)\right)^{(m)}.$$

By (2.6), $\Delta^k \left((-1)^k R^e_{2k}(x)\right) * u(x) = \delta * u(x) = (-1)^k R^e_{2k}(x) * \left(R^H_{2(k-1)}(v)\right)^{(m)}$.
It follows that

$$u(x) = (-1)^k R^e_{2k}(x) * \left(R^H_{2(k-1)}(v)\right)^{(m)}. \tag{2.13}$$

3 Main results

Theorem Given The equation

$$\diamondsuit^k u(x) = f(x) \tag{3.1}$$

where $\diamondsuit^k$ is the Diamond operator iterated k-times defined by (1.1), $f(x)$ is a generalized function, $u(x)$ is an unknown generalized function and $x = (x_1, x_2, \ldots x_n) \in R^n$-the n-dimensional Euclidean space and n is even, then (3.1) has the general solution

$$u(x) = (-1)^k R^e_{2k}(x) * \left(R^H_{2(k-1)}(v)\right)^{(m)} + (-1)^k K_{2k,2k}(x) * f(x) \tag{3.2}$$

where $\left(R^H_{2(k-1)}(v)\right)^{(m)}$ is a function with m-derivatives defined by (2.1) and $K_{2k,2k}(x)$ is defined by (1.6) with $\alpha = \beta = 2k$.

Proof Convolving (3.1) both sides by $(-1)^k K_{2k,2k}(x)$, we obtain

$$(-1)^k K_{2k,2k}(x) * \diamondsuit^k u(x) = (-1)^k K_{2k,2k}(x) * f(x).$$

By (1.4) $\diamondsuit^k \left((-1)^k K_{2k,2k}(x)\right) * u(x) = \delta * u(x) = (-1)^k K_{2k,2k}(x) * f(x)$. We obtain $u(x) = (-1)^k K_{2k}(x) * f(x)$. Since, for a Homogeneous equation $\diamondsuit^k u(x) = 0$ we have a solution $u(x) = (-1)^k R^e_{2k}(x) * \left(R^H_{2(k-1)}(v)\right)^{(m)}$.

Thus the general solution of (3.1) is

$$u(x) = (-1)^k R^e_{2k}(x) * \left(R^H_{2(k-1)}(v)\right)^{(m)} + (-1)^k K_{2k,2k}(x) * f(x).$$

In particular, if $q = 0$ the equation (3.1) becomes the Laplace equation $\triangle^{2k}u(x) = f(x)$ where $x = (x_1, x_2, x_3, ..., x_p) \in R^p$ and p is even. Using the formulae $\Gamma(2z) = 2^{2z-1}\pi^{-1/2}\Gamma(z)\Gamma(z+\frac{1}{2})$ and $\Gamma(\frac{1}{2}+z)\Gamma(\frac{1}{2}-z) = \pi sec(\pi z)$. Then for $\alpha = 2k$ the function of (2.1) becomes $(-1)^k R^e_{2k}(x)$ where $R^e_{2k}(x)$ is defined by (2.5) and $x = (x_1, x_2, ..., x_p) \in R^p$. Thus by (1.6)

$$\begin{aligned}(-1)^k K_{2k,2k}(x) &= (-1)^k R^e_{2k}(x) * (-1)^k R^e_{2k}(x) \\ &= R^e_{4k}(x) \text{ see ([2], p156-159)}\end{aligned}$$

where $x = (x_1, x_2, ..., x_p) \in R^p$ and p is even.

Now, from (2.12) for $q = 0$ we have

$$\begin{aligned}u(x) &= (-1)^k R^e_{2k}(x) * (-1)^{k-1}\left(R^e_{2(k-1)}(x)\right)^{(m)} \\ &= (-1)^{2k-1}\left(R^e_{4k-2}(x)\right)^{(m)} \quad \text{for } x = (x_1, x_2, ..., x_p) \in R^p.\end{aligned}$$

Thus the equation (3.2) becomes

$$u(x) = (-1)^{2k-1}\left(R^e_{4k-2}(x)\right)^{(m)} + R^e_{4k}(x) * f(x) \tag{3.3}$$

for $x = (x_1, x_2, ..., x_p) \in R^p$ and p is even.
It follows that (3.3) is the general solution of the Laplace equation $\triangle^{2k}u(x) = f(x)$ where $\triangle^{2k}$ is the Laplace operator iterated $2k$-times defined by (1.3) for $x = (x_1, x_2, ..., x_n) \in R^n$ and n is even.

Now consider the case for the Wave Equation. Given the equation

$$\Box^k V(x) = f(x) \tag{3.4}$$

where $f(x)$ is a generalized function,$\Box^k$ is defined by (1.2) and $V(x)$ is an unknown function. By ([5],p11) we obtain $V(x) = R^H_{2k}(v) * f(x)$ is a solution of (3.4) where $R^H_{2k}(v)$ is defined by (2.1).

Now, from (3.1) we have $u(x) = (-1)^k K_{2k,2k}(x) * f(x)$ is a solution where $K_{2k,2k}(x)$ is defined by (1.6) with $\alpha = \beta = 2k$ or

$$u(x) = \left[(-1)^k R^e_{2k}(x) * R^e_{2k}(v)\right] * f(x) \tag{3.5}$$

Convolving both sides of (3.5) by $(-1)^k R^e_{-2k}(x)$, we obtain

$$\begin{aligned}(-1)^k R^e_{-2k}(x) * u(x) &= \left((-1)^{2k} R^e_{-2k}(x) * R^e_{2k}(x)\right) * R^H_{2k}(v) * f(x) \\ &= \left(R^e_0(x) * R^H_{2k}(v)\right) * f(x) \\ &= \left(\delta * R^H_{2k}(v)\right) * f(x) \\ &= R^H_{2k}(v) * f(x) \quad \text{see ([2],p156-159)}\end{aligned}$$

Thus it follows that

$$V(x) = (-1)^k R^e_{-2k}(x) * u(x) \tag{3.6}$$

In particular, for $k = 1$, we obtain $V(x) = R^H_2(v) * f(x)$ is a solution of the equation

$$\Box V(x) = f(x). \tag{3.7}$$

If we put $p = 1$ and $x_1 = t$(time),then $\Box = \frac{\partial^2}{\partial t^2} - \sum_{i=2}^n \frac{\partial^2}{\partial x_i^2}$ is the wave operator. Thus (3.7) becomes wave equation,

$$\left(\frac{\partial^2}{\partial t^2} - \sum_{i=2}^{n} \frac{\partial^2}{\partial x_i^2}\right) V(x) = f(x) \tag{3.8}$$

Thus $V(x) = M_2(v) * f(x)$ is a solution of (3.8) and the general solution of (3.8) is $V(x) = \delta^{(m)}(v) + M_2(v) * f(x)$ where $\delta^{(m)}(v)$ is a solution for $f(x) = 0$ $v = t^2 - x_2^2 - x_3^2 - \cdots - x_n^2$ and $M_2(v)$ is defined by (2.4) with $v = t^2 - x_2^2 - x_3^2 - \cdots - x_n^2$.

Now in (3.1),put $k = 1$ and by (3.2) we obtain

$$\begin{aligned} u(x) &= (-1)R^e_2(x) * \left(R^H_0(v)\right)^{(m)} + (-1)K_{2,2}(x) * f(x) \\ &= (-1)R^e_2(x) * \delta^{(m)}(v) + (-1)K_{2,2}(x) * f(x) \end{aligned} \tag{3.9}$$

is a solution of the equation $\Diamond u(x) = f(x)$ and by (3.6) with $k = 1, V(x) = (-1)R^e_{-2}(x) * u(x)$ is a solution of (3.7) where $u(x)$ is defined by (3.9). Thus

$$\begin{aligned} V(x) &= (-1)R^e_{-2}(x) * ((-1)R^e_2(x) * \delta^{(m)}(v)) \\ &\quad +(-1)R^e_{-2}(x) * ((-1)K_{2,2}(x) * f(x)) \\ &= \left(R^e_{-2}(x) * R^e_2(x)\right) * \delta^{(m)}(v) \\ &\quad +(R^e_{-2}(x) * R^e_2(x)) * R^H_2(x) * f(x) \\ &= R^e_0(x) * \delta^{(m)}(v) + R^e_0(x) * (R^H_2(x) * f(x)) \\ &= \delta^{(m)}(v) + R^H_2(x) * f(x) \qquad (R^e_0(x) = \delta) \end{aligned} \tag{3.10}$$

where $v = x_1^2 + x_2^2 + \cdots + x_p^2 - x_{p+1}^2 - x_{p+2}^2 - \cdots - x_{p+q}^2,\ p + q = n$.
Now, if we put $p = 1$ and $x_1 = t$, then (3.10) becomes $V(x) = \delta^{(m)}(v) + M_2(v) * f(x)$ since $R^H_2(x)$ becomes $M_2(v)$ for $v = t^2 - x_2^2 - x_3^2 - \cdots - x_n^2$ where $M_2(v)$ is defined by (2.4) with $\alpha = 2$. Thus $V(x) = \delta^{(m)}(v) + M_2(v) * f(x)$ is the general solution of the wave equation (3.8) and $\delta^{(m)}(v)$ is a solution of

$$\left(\frac{\partial^2}{\partial t^2} - \sum_{i=2}^{n} \frac{\partial^2}{\partial x_i^2}\right) V(x) = 0 \tag{3.11}$$

Now $v = t^2 - x_2^2 - x_3^2 - \cdots - x_n^2$, let $r^2 = x_2^2 + x_3^2 + \cdots + x_n^2$. Thus by ([1],p234-236) we obtain $V(x,t) = \delta^{(m)}(t^2 - r^2)$ is the solution of (3.11) with the initial conditions $V(x,0) = 0$ and $\frac{\partial V(x,0)}{\partial t} = (-1)^m 2\pi^{m+1}\delta(x)$ at $t = 0$ and $x = (x_2, x_3, \ldots, x_n) \in R^{n-1}$.

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