ตัวแผ่กระจายสองมิติแบบแม่นตรงของอิเล็กตรอนในสนามแม่เหล็กและสนามไฟฟ้าศักย์สุ่มแบบควอดราติก

นายอนุศิษฎ์ ทองนำ

สถาบันวิทยบริการ
จุฬาลงกรณ์มหาวิทยาลัย

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EXACT TWO-DIMENSIONAL PROPAGATOR OF AN ELECTRON IN MAGNETIC AND ELECTRIC FIELDS WITH A QUADRATIC RANDOM POTENTIAL

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อนุศิษฏ์ ทองนำ : ตัวแผ่กระจายสองมิติแบบแม่นตรงของอิเล็กตรอนในสนามแม่เหล็กและสนามไฟฟ้าศักย์สุ่มแบบควอดราติก. (EXACT TWO-DIMENSIONAL PROPAGATOR OF AN ELECTRON IN MAGNETIC AND ELECTRIC FIELDS WITH A QUADRATIC RANDOM POTENTIAL). อ.ที่ปรึกษา: รศ. ดร. วิชิต ศรีตระกูล, อ. ที่ปรึกษาร่วม : ศ. ดร. วิรุฬห์ สาย - คณิต จำนวนหน้า 78 หน้า. ISBN 974-17-3692-4.

ตัวแผ่กระจายสองมิติแบบแม่นตรงของอิเล็กตรอนในสนามแม่เหล็กตามขวางและสนามไฟฟ้าเปลี่ยนตามเวลากับศักย์สุ่มแบบนอนโลคอลฮาโมนิคของหนึ่งตัวแปร ได้ถูกคำนวณโดยใช้วิธีการอินทิเกรตตามวิถีของฟาน์ยแมน โดยพิจารณาวิธีการแปลงแบบสตราโตโนวิชและเมตริกซ์ 2x2 ในวิทยานิพนธ์นี้เราเสนอแบบจำลองของศักย์สุ่มแบบนอนโลคอลฮาโมนิคของสองตัวแปร สำหรับตัวแผ่กระจายสองมิติแบบแม่นตรงในสนามแม่เหล็กตามขวางและสนามไฟฟ้าพร้อมด้วยศักย์แบบนอนโลคอลฮาโมนิคของสองตัวแปรไม่สามารถคำนวณอย่างแม่นตรง อย่างไรก็ตามเราสามารถคำนวณหาตัวแผ่กระจายวิเคราะห์โดยแยกลากรางเจียนเป็นสองส่วน ในส่วนแรกสามารถคำนวณอย่างแม่นตรงโดยใช้วิธีแบบจำลองของสองอนุภาค ส่วนที่สองคำนวณด้วยการประยุกต์วิธีการประมาณแบบคิวมูแลนต์ลำดับที่หนึ่ง ความหนาแน่นสถานะของศักย์สุ่มแบบเกาส์เซียนถูกคำนวณด้วยวิธีการแปรผันตามวิถีที่ขอบเขตพลังงานต่ำและสูงตามลำดับ เราเปรียบเทียบความหนาแน่นสถานะที่ได้กับผลลัพธ์ของทฤษฎีหนึ่งตัวแปรและผลลัพธ์ของการจำลองแบบยึดแน่นที่ขอบเขตแบบไวท์นอยส์

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ANUSIT THONGNUM : EXACT TWO-DIMENSIONAL PROPAGATOR OF AN ELECTRON IN MAGNETIC AND ELECTRIC FIELDS WITH A QUADRATIC RANDOM POTENTIAL. THESIS ADVISOR : ASSOC. PROF. WICHIT SRITRAKOOL, Ph.D. THESIS CO-ADVISOR : PROF. VIRULH SA-YAKANIT, F.D, 78 pp. ISBN 974-17-3692-4.

The exact two-dimensional propagator of an electron moving in a transverse magnetic field and a time-varying electric field with a one-parameter nonlocal harmonic random potential was calculated exactly using the Feynman path integral method by considering the Stratonovich's transformation and the 2x2 matrices methods. In this thesis, we introduce the nonlocal harmonic random potential with two parameters. The exact two-dimensional propagator in a transverse magnetic field and an electric field with a two-parameter nonlocal harmonic potential cannot be calculated exactly. However, we can evaluate the analytic propagator by separating the Lagrangian into two parts. The first part can be calculated exactly by the two-particle model method. The second part can be calculated by first-order cumulant approximation. The density of states with a Gaussian random potential can be calculated by the variational path integral method in the low and high energy limits, respectively. In addition, we compare the density of states with the one-parameter theory and the tight-binding simulation result in the white noise limit.

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Chapter 1
Introduction

The standard formulation of quantum mechanics was developed by Schrödinger, Heisenberg and others in the 1920s. Those two formulations were shown by Dirac to be equivalent. These approaches are based on the Hamiltonian of a system, which is a function of operator. The third formulation, Feynman path integral developed by R. P. Feynman, is based on the Lagrangian of the system. This approach was inspired by P. A. M. Dirac's [2], remarks that the action plays a central role in classical mechanics. Feynman forwarded the idea by postulating that not classical path contributes but all possible paths. The central concept in Feynman's approach is the propagator, containing all the information about the system. In 1955, Feynman [3] applied the path integral to the polaron problem by calculating the self energy and the effective mass of the polaron. The result was valid for an arbitrary coupling strength (α) of electron-phonon interactions. Consequently, path integrals have been applied widely to other problems and various fields of theoretical physics.

In the meantime, path integrals have been applied intensively to the theory of disordered systems. First, Edwards and Gulayev [4] introduced the path integral to an electron moving in random scatterers but the density of states cannot be solved explicitly. However, Sa-yakanit [5], and Sa-yakanit and Glyde [6] used the variational path integral to calculate the density of states in the above cases, i.e., the Gaussian potential and the screened Coulomb potential. Later, Bezak [7] derived the action of an electron gas in a random potential and expanded the autocorrelation function of Edwards' model at very large correlation

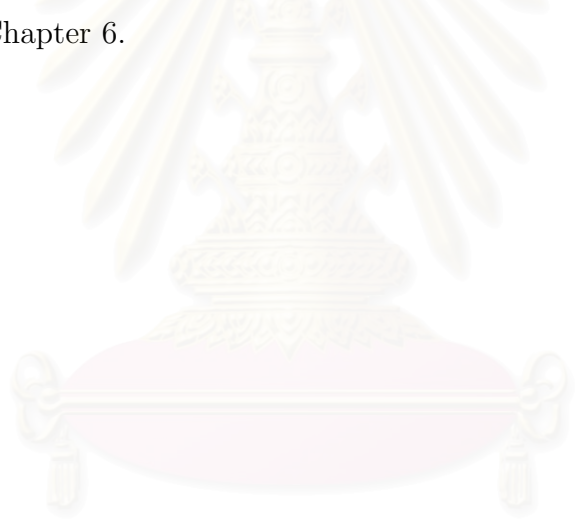
length. The theory of Bezak introduced the autocorrelation function by using a nonlocal harmonic oscillator that represents an average potential energy. The exact propagator can be applied to calculate the density of states at the limit of the band-tail energy ($E \to -\infty$). This model has also been applied to other problems of disordered systems. Finally, the two-particle model was introduced by Sa-yakanit [8]. The action is an electron moving in a two-parameter nonlocal harmonic random potential with the force constant (κ) and the harmonic frequency (ω). The action is exactly identical to the polaron trial action using by Osaka [9], but substituting of a real time variable by the imaginary time ($t \to -i\hbar\beta$).

For a system of non-interacting electrons confined in two-dimensions under the influence of a transverse magnetic field, an electron occupies a discrete level known as the Landau level [10]. If we apply an electric field to a three-dimensional system, an electron can move freely along the direction of the electric field with the corresponding classical orbit being a helix. In real systems, in which impurities are present, each Landau level is broadened into the band, which is called "Landau band" [11]. The state of electron in Landau band consists of the extended (delocalized) state and the localized state [12]. This gives rise to the quantum Hall effect [13], discovered by von Klitzing in 1980.

The purpose of this thesis is to introduce the two-parameter nonlocal harmonic random potential in the method. The main calculation is the two-dimensional propagator of an electron in a two-parameters nonlocal harmonic potential energy with transverse magnetic and x-direction electric fields, and the density of states of a Gaussian random system.

The outline of this thesis is as follows : in the next Chapter, we review the basic idea of the Feynman path integral and the derivation of Feynman propaga-

tor, the semi-classical approximation and the general quadratic Lagrangian. The examples are shown in the last section. In Chapter 3, we review the mathematical models of a random potential via the path integral formulation. In Chapter 4, we calculate the two-dimensional propagator of an electron in a two-parameter nonlocal harmonic random potential with transverse magnetic and x-direction electric fields. In Chapter 5, the density of states in two-dimensional random system is calculated using the approximation in the low-energy and the high-energy limits. The normalized density of states is then compared with the result of the tight-binding simulation in the white noise limit. Finally, the conclusions is presented in Chapter 6.



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Chapter 2
Feynman's Path Integrals

The Feynman path integral provides us an approach to solve quantum mechanic problems, based on a Lagrangian of the system. The most important thing of Feynman's approach is the propagator, which is a Green's function of Schrödinger equation or the superposition of probability amplitudes in general representation, containing all the information about the system. Furthermore, the propagator also means the sum of contributions from all paths. However, in certain cases, the sum over all contribution paths can be approximated to be contribution of the classical path. This approximation is called the semi-classical approximation based on an expansion around the classical path.

2.1 Derivation of Feynman's Propagators

2.1.1 The Superposition of Probability Amplitudes

In quantum mechanics, the central quantity is the propagator (K). The propagator represents the quantum mechanical transition amplitude defined by $K(x'', t''; x', t') \equiv \langle x'', t''|x', t'\rangle$. The right hand side bracket means that the system will be found at position x'' at time t'' when the position x' and time t' are specified. This definition is obtained by the postulation of the interference phenomena in quantum mechanics, obeying the composition law.

We begin with discussion of probability amplitudes in quantum mechanics in general representation, which is the Green's function of time-dependent Schrödinger equation. First, let us begin with the time-dependent Schrödinger

equation,

$$\left[i\hbar\frac{\partial}{\partial t}-\hat{H}\right]\Psi(x,t)=0, \tag{2.1}$$

where the Hamiltonian is defined by

$$H=\frac{p^2}{2m}+V(x). \tag{2.2}$$

We can define the one-electron Green function of this equation as the solution of

$$\left[i\hbar\frac{\partial}{\partial t}-\hat{H}\right]g(x^{''},t^{''};x^{'},t^{'})=\delta(x^{''}-x^{'})\delta(t^{''}-t^{'}). \tag{2.3}$$

As we have known, the propagator can be defined by a transition amplitude, then

$$K(x^{''},t^{''};x^{'},t^{'})\equiv g(x^{''},t^{''};x^{'},t^{'})=\langle x^{''}|\exp\{-i\hat{H}(t^{''}-t^{'})/\hbar\}|x^{'}\rangle. \tag{2.4}$$

The one-dimensional time-dependent Green function of Schrödinger equation can be represented in a matrix form, which is an expression of the Feynman propagator. First, we consider the exponential of Hamiltonian operator for any N times

$$e^{-i\hat{H}t/\hbar}=[e^{-i\hat{H}t/N\hbar}]^N. \tag{2.5}$$

We define the small subinterval time as

$$\epsilon=\frac{t}{N}, \tag{2.6}$$

and consider the limit $N\to\infty$ that $t_{i+1}-t_i=\epsilon$. Now we can write

$$\langle x^{''},t^{''}|x^{'},t^{'}\rangle=\langle x^{''}|\underbrace{e^{-i\hat{H}(t_N-t_{N-1}+t_{N-1}\ldots+t_1-t_0)/\hbar}}_{(N)-times}|x^{'}\rangle$$

$$= \langle x^{''}|e^{-i\hat{H}(\epsilon+\epsilon+\epsilon+...)/\hbar}|x^{'}\rangle. \tag{2.7}$$

From the Baker-Haudoff lemma the transition amplitude is reduced to

$$\langle x^{''}, t^{''}|x^{'}, t^{'}\rangle = \langle x^{''}|e^{-i\hat{H}\epsilon/\hbar}.e^{-i\hat{H}\epsilon/\hbar}...e^{-i\hat{H}\epsilon/\hbar}|x^{'}\rangle. \tag{2.8}$$

We insert the completeness relation of $N-1$ intermediate space-time coordinates $(x_1, x_2, x_3, ..., x_{N-1})$ into the transition amplitude, then we obtain

$$\langle x^{''}, t^{''}|x^{'}, t^{'}\rangle = \int dx_1...dx_{N-1}\langle x^{''}|e^{-i\hat{H}\epsilon/\hbar}|x_{N-1}\rangle\langle x_{N-1}|e^{-i\hat{H}\epsilon/\hbar}|x_{N-2}\rangle..\langle x_1|e^{-i\hat{H}\epsilon/\hbar}|x^{'}\rangle. \tag{2.9}$$

We consider the matrix element, the exponential involving the Hamiltonian operator. If the operator acts on the eigenstate, then it gives the eigenvalue. Thus, the matrix element becomes

$$\langle x_n|\exp(\frac{-i\epsilon}{\hbar}[\frac{\hat{p}^2}{2m} + \hat{V}(x)])|x_{n-1}\rangle = \langle x_n|\exp[-\frac{i\epsilon}{2m\hbar}\hat{p}^2]|x_{n-1}\rangle\exp[-i\epsilon V(x_{n-1})/\hbar]. \tag{2.10}$$

The next step, we introduce the completeness relation of momentum space

$$\int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}|p\rangle\langle p| = 1, \tag{2.11}$$

and the momentum eigenfunction for a free particle

$$\langle x|p\rangle = \exp\left(\frac{ipx}{\hbar}\right) \tag{2.12}$$

and substitute the identities into the matrix element of equation (2.10), then

$$\int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}\langle x_n|\exp(-\frac{i\epsilon}{2m\hbar}\hat{p}^2)|p\rangle\langle p|x_{n-1}\rangle\exp[-i\epsilon V(x_{n-1})/\hbar]$$

$$= \exp[-i\epsilon V(x_{n-1})/\hbar] \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \exp\left[-\frac{i\epsilon p^2}{2m\hbar} + \frac{i}{\hbar}(x_n - x_{n-1})p\right]. \tag{2.13}$$

From the Gaussian integral formula

$$\int_{-\infty}^{\infty} dp e^{-ap^2+bp} = \sqrt{\frac{\pi}{a}} e^{-\frac{b^2}{4a}}, \tag{2.14}$$

the matrix element in equation (2.13) can be reduced to

$$\langle x_n| \exp(\frac{-i\epsilon}{\hbar}[\frac{p^2}{2m} + V(x)])|x_{n-1}\rangle = \sqrt{\frac{m}{2\pi i\hbar\epsilon}} \exp\left[\frac{im\epsilon}{2\hbar}(\frac{x_n - x_{n-1}}{\epsilon})^2 - \frac{i\epsilon}{\hbar}V(x_{n-1})\right]. \tag{2.15}$$

The matrix element is an independent operator. We substitute the matrix element in equation (2.15) into equation (2.9). For every matrix element we obtain the transition amplitude

$$\langle x'', t''|x', t'\rangle = (\frac{m}{2\pi i\hbar\epsilon})^{N/2} \int dx_1 ... dx_N \exp\frac{i}{\hbar} \sum_n \left[\frac{m\epsilon}{2}(\frac{x_n - x_{n-1}}{\epsilon})^2 - \epsilon V(x_{n-1})\right]. \tag{2.16}$$

Consider the infinitesimal time interval, we should be able to obtain the transition amplitude for a finite time interval as

$$\langle x'', t''|x', t'\rangle = \int \prod_{n=1}^{N} (\frac{m}{2\pi i\hbar\epsilon})^{1/2} dx_n \exp\frac{i\epsilon}{\hbar} \sum_{n=1}^{N} \left[\frac{m}{2\epsilon^2}(x_n - x_{n-1})^2 - V(x_{n-1})\right]. \tag{2.17}$$

At the continuum notation or the infinitesimal time interval approach to zero, the transition amplitude or the Feynman propagator can be rewritten as

$$K(x^{''},t^{''};x^{'},t^{'}) \equiv \langle x^{''},t^{''}|x^{'},t^{'}\rangle = \int D[x(t)] \exp\frac{i}{\hbar}\left(\int_{t'}^{t^{''}}\left[\frac{m}{2}\dot{x}^2(t) - V(x)\right]dt\right), \tag{2.18}$$

where the integral measure

$$\int D[x(t)] = \lim_{\epsilon\to 0}\int\prod_{n=1}^{N}(\frac{m}{2\pi i\hbar\epsilon})^{1/2}dx_n, \tag{2.19}$$

and the action

$$S[x(t)] = \int_{t'}^{t^{''}} dtL(x,\dot{x},t). \tag{2.20}$$

This is the Feynman path integrals expression form derived by the time-dependent Green function of Schrödinger equation.

2.1.2 The Sum Over All Paths

In classical mechanics, when a particle moves from one point to another point. From the principle of least action, a particle has only one classical path that is stationary. Thus the action S is a minimum value

$$\delta S = 0. \tag{2.21}$$

We can say that the value of S is unchanged if the path $x(t)$ is the classical path. The action function can be defined by

$$S = \int_{t'}^{t^{''}} dtL(\dot{x},x,t), \tag{2.22}$$

where L is Lagrangian of the system. In other words, the principle of least action is the Lagrange equation.

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Nevertheless, the important concept of quantum mechanics is probability. If we specify the position of a particle, then we cannot specify the momentum of a particle. Therefore, we cannot predict the path in which a particle can take. In the 1950 Feynman [1] introduced the theory of sum over all paths. In a sense, if a particle moves from point $x^{'}$ at initial time $t^{'}$ to the end point $x^{''}$ at time $t^{''}$, there are many possible paths in which a particle can take. Thus a particle moves with the action function of possible paths. We may summarize Feynman's postulation as

I. If an ideal measurement is performed determine whether a particle has a path lying in a region of space-time, then the probability that the result will be affirmative is the absolute square of a sum of complex contributions, one form each path in the region.

II. The paths contribute equally in magnitude, but the phase of their contribution is classical action $S[x(t)]$ in unit of $\hbar$.

This postulation, the probability of particle to go from a point $x^{'}$ at time $t^{'}$ to the point $x^{''}$ at $t^{''}$ is the absolute square of the propagator,

$$P(x^{''}, x^{'}) = |K(x^{''}, t^{''}; x^{'}, t^{'})|^2. \tag{2.23}$$

that the propagator is the sum of contribution from each path. Therefore, the propagator can be written

$$K(x^{''}, t^{''}; x^{'}, t^{'}) = \sum_{overall paths from x^{'} to x^{''}} \Phi[x(t)], \tag{2.24}$$

where Φ is the contribution of path in which proportional to the action S,

$$\Phi[x(t)] = (cont) \exp\left(\frac{i}{\hbar} S[x(t)]\right). \tag{2.25}$$

We construct the path by connecting all the points so selected with straight line of a point on space time coordinate. We choose a subset of all paths by first separating the independent time in to small interval, ϵ. This gives us a set of successive time $t_i\{t_1, t_2, t_3, ...\}$ between the values $t^{'}$ to $t^{''}$, where $t_{i+1} = t_i + \epsilon$. At each time, t_i, we select some special point x_i and constructing a path by connecting all of the point, so we set the form of them to be a line. This processes are shown in Figure 2.1. It is possible to define a sum over all paths constructed in this manner by taking a multiple integral over all values of x_i for i from 1 to $n-1$, where

$$t_a = t^{'}, t_b = t^{''}, n\epsilon = t^{''} - t^{'}$$

$$x_a = x^{'}, x_b = x^{''}.$$

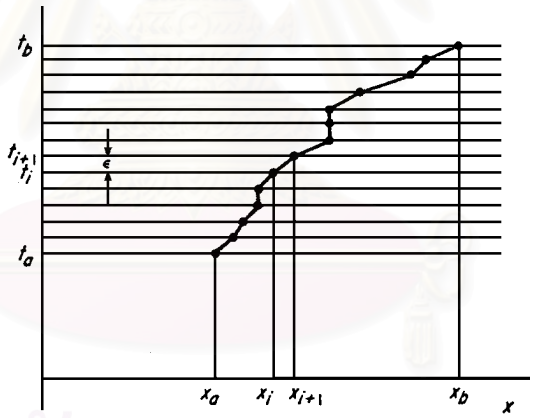

Figure 2.1 Diagram showing how the path integrals can be constructed [25].

By using this method, equation (2.24) becomes

$$K(x^{''}, t^{''}; x^{'}, t^{'}) \approx \int\int ... \int dx_1 dx_2 ... dx_{n-1} \Phi[x(t)] \tag{2.26}$$

or

$$K(x^{''},t^{''};x^{'},t^{'}) \approx \int\int ... \int dx_1 dx_2 ... dx_{n-1}(const) \exp \frac{i}{\hbar} S[x(t)]. \tag{2.27}$$

We do not integrate x_0 or x_n because these are the fixed end point $x^{'}$ and $x^{''}$. In order to achieve the correct measure, equation (2.27) must be taken in the limit $\epsilon \to 0$ and some normalizing factor A^{-1} which depends on ϵ must be provided in in order that the limit of equation (2.27) becomes

$$K(x^{''},t^{''};x^{'},t^{'}) = \lim_{\epsilon \to 0} \frac{1}{A} \int\int ... \int \frac{dx_1}{A} \frac{dx_2}{A} ... \frac{dx_N}{A} \exp \frac{i}{\hbar} S[x(t)], \tag{2.28}$$

where a normalization constant

$$A = (\frac{m}{2\pi i \hbar T})^{1/2}. \tag{2.29}$$

Equation (2.28) can also be written in a less restrictive notation as

$$K(x^{''},t^{''};x^{'},t^{'}) = \int D[x(t)] \exp \frac{i}{\hbar} S[x(t)]. \tag{2.30}$$

This is called a path integral (sum over all paths) and the amplitude $K(x^{''},t^{''};x^{'},t^{'})$ is known as the Feynman propagator. We see that the propagator followed Feynman's argument has exactly the same form as the time-dependent Green function (the superposition of probability amplitudes).

2.2 The Semi-Classical Approximation

The semi-classical approximation is applied by the path integral. The classical path from $x^{'}$ to $x^{''}$ is denoted by $\bar{x}(t)$. We express an arbitrary path in terms of $x(t)$ as $x(t) = \bar{x}(t) + \delta x(t)$. In general we are simply shifting the variable

$x(t)$ by $\bar{x}(t)$ with the new variable $\delta x(t)$. An arbitrary path can be expressed in terms of $\bar{x}(t)$ and $\delta x(t)$ by expanding the Taylor's series of $V(\bar{x}+\delta x)$. We can write the action as

$$\begin{aligned} S &= \int_{t'}^{t''} dt \left\{ \frac{m}{2}(\frac{d}{dt}(\bar{x}+\delta x))^2 - V(\bar{x}+\delta x) \right\} \\ &= \int_{t'}^{t''} dt \left\{ \frac{m}{2}[\frac{d^2\bar{x}}{dt^2} + 2m\frac{d\bar{x}}{dt}\frac{d\delta x}{dt} + (\frac{d\delta x}{dt})^2] - V(\bar{x}+\delta x) \right\} \\ &= S_c + \int_{t'}^{t''} dt\{m\frac{d\bar{x}}{dt}\frac{d\delta x}{dt} - \frac{1}{2}\frac{\partial V}{\partial \bar{x}}\delta x\} \\ &\quad + \int_{t'}^{t''} dt\{\frac{m}{2}(\frac{d}{dt}\delta x)^2 - \frac{1}{2}\frac{\partial^2 V}{\partial \bar{x}^2}(\delta x)^2\} \\ &\quad + \int_{t'}^{t''} dt\{-\frac{1}{6}\frac{\partial^3 V}{\partial \bar{x}^3}(\delta x)^3 + ...\}. \end{aligned} \tag{2.31}$$

Classifying terms by their order in $\delta x(t)$, we can write

$$S = S_c + S^{(2)} + S^{(3)} + ..., \tag{2.32}$$

where there is no term linear in $\delta x(t)$ because $\bar{x}(t)$ satisfies the equation of motion and $\delta x(t)$ vanishes at the end points. The semi-classical approximation to the path integral involves dropping all terms higher than the quadratic in $\delta x(t)$. From the expression for the Feynman path integral, then

$$K(x'', t''; x', t') = \exp\{i\frac{S_c}{\hbar}\} \int_{t'}^{t''} D\delta x(t) \exp\{i\frac{S^{(2)}}{\hbar}\}, \tag{2.33}$$

where we neglect higher order, explicitly $S^{(2)}$ is the phase difference between the classical path and contribution paths as

$$S^{(2)} = \int_{t'}^{t''} dt\{\frac{m}{2}(\frac{d}{dt}\delta x)^2 - \frac{1}{2}\frac{\partial^2 V}{\partial \bar{x}^2}(\delta x)^2\}. \tag{2.34}$$

However, it is possible to express the answer for the Gaussian integral over $\delta x(t)$ in terms of the classical action S_c called the Van-Vleck Pauli formula [14,15,16],

$$K(x^{''},t^{''};x^{'},t^{'}) = \sqrt{\frac{1}{2\pi i\hbar}(-\frac{\partial^2 S_c}{\partial x_{t'}\partial x_{t''}})}\exp\{i\frac{S_c}{\hbar}\}. \tag{2.35}$$

For more variables, the pre-factor involves the determinant of the matrix of derivatives of S_c in the d-dimensions. The semi-classical approximation can be used with good results for a smooth potential. However, the formula breaks down on the caustic where the Van Vleck-Pauli determinant vanishes.

2.3 The General Quadratic Lagrangian

From a previous section, the method of direct integration can be carried out for the the path integral. For the fluctuation potential case, the semi-classical approximation is more difficult to work out because it breaks down on a Gaussian integral. In this section we show that the quadratic Lagrangian is the general method to direct integrating out of path integrals. The two cases of general quadratic Lagrangian are the quadratic Lagrangian (semi-classical approximation) and the two-time quadratic Lagrangian (fluctuation potential case).

2.3.1 The Quadratic Lagrangian

We know from classical physics that the action S is extremized and then it furnishes us the classical path is completely fixed. Therefore, any path $x(t)$ can be written in terms of the classical path $\bar{x}(t)$ and a new variable $y(t)$. That is

$$x(t) = \bar{x}(t) + y(t), \tag{2.36}$$

and the integral measurement $D[x(t)]$ can replaced by $D[y(t)]$. This means that a point on the path by its distance $x(t)$ from an arbitrary coordinate axis, we now

define it by its derivation $y(t)$ from the classical path, as shown in Figure 2.2. Since any path $x(t)$ and the classical path $\bar{x}(t)$ must have the same end points. The condition which the derivations $y(t)$ have to satisfy is $y(t') = y(t'') = 0$.

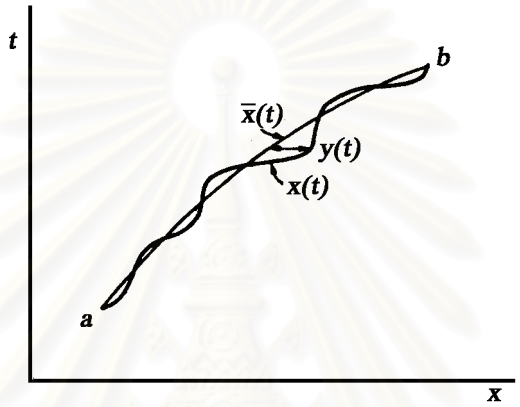

Figure 2.2 Diagram showing a path deviating from the classical path [25].

The Lagrangian will be the quadratic form

$$L = a(t)\dot{x}^2(t) + b(t)\dot{x}(t)x(t) + c(t)x^2(t) + d(t)\dot{x}(t) + e(t)x(t) + f(t). \tag{2.37}$$

Hence, the action S can be expressed as

$$\begin{aligned} S[x(t)] &= S[\bar{x}(t) + y(t)] \\ &= \int_{t'}^{t''} \left[a(t)\left\{\dot{\bar{x}}^2(t) + 2\dot{\bar{x}}(t)\dot{y}(t) + \dot{y}^2(t)\right\} + ... + f(t)\right] dt. \end{aligned} \tag{2.38}$$

It is obvious that the integral of all terms involving exclusively $\bar{x}(t)$ is exactly the classical action and the integral of all terms that are linear in $y(t)$ precisely

vanishes from boundary condition. So, all the remaining terms in the integral are the second-order terms in $y(t)$ only. That is

$$S[x(t)] = S_{cl}[\bar{x}(t)] + \int_{t'}^{t''} \left[a(t)\dot{y}^2(t) + b(t)\dot{y}(t)y(t) + c(t)y^2(t)\right] dt. \tag{2.39}$$

Thus the propagator is the integral over paths $y(t)$ does not depend upon the classical path and all paths $y(t)$ start from and return to the point $y = 0$, can be written as

$$K(x'', t''; x', t') = \exp\left(\frac{i}{\hbar} S_{cl}[\bar{x}(t)]\right) N \int_0^0 D[y(t)] \exp\left\{\frac{i}{\hbar}\int_{t'}^{t''} dt[a(t)\dot{y}^2(t) + b(t)\dot{y}(t)y(t) + c(t)y^2(t)]\right\}. \tag{2.40}$$

For the quadratic Lagrangian, the propagator can be written as

$$K(x'', t''; x', t') = F(T) \exp\left\{\frac{i}{\hbar} S_{cl}[\bar{x}(t)]\right\}, \tag{2.41}$$

where the prefactor is

$$F(T) = N \int_0^0 D[y(t)] \exp\left\{\frac{i}{\hbar}\int_{t'}^{t''} dt[a(t)\dot{y}^2(t) + b(t)\dot{y}(t)y(t) + c(t)y^2(t)]\right\}. \tag{2.42}$$

For the quadratic Lagrangian, it can be seen that the path integral in equation (2.40) which is a product of two functions, one of which does not depend upon the end-point positions. This propagator is similar to the semi-classical approximation.

2.3.2 The Two-Time Quadratic Lagrangian

Such a situation with an electron interacting with a larger system, Feynman [3] was first to introduce a nonlocal action in the polaron problem. The general form of two-time Lagrangian is

$$L = \frac{m}{2}\dot{x}^2(t) - \frac{1}{2}\int_0^T dsG(t,s)x(t)x(s). \tag{2.43}$$

Physically $G(t,s)$ is a simple phenomenological memory effect which arises when the system interacts with a larger system. The example of this problem is an electron moving in a disorder system or a random potential. The propagator is very similar to the quadratic action. Thus, the entire contribution to the propagator comes from the classical path alone

$$K(x'',t'';x',t') = F(T)\exp\left\{\frac{i}{\hbar}S_{cl}[x(t)]\right\}, \tag{2.44}$$

where the prefactor is

$$F(T) = N\int_0^0 D[x(t)]\exp\left\{\frac{i}{\hbar}S_{cl}\right\}. \tag{2.45}$$

2.4 Examples

2.4.1 The Harmonic Oscillator

For a simple problem is the one-dimensional harmonic oscillator. The Lagrangian is given by

$$L(x,\dot{x}) = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2x^2. \tag{2.46}$$

From the semi-classical approximation, the propagator can be expressed in the form

$$K(x_2,t_2;x_2,t_1) = F(T)\exp\{\frac{i}{\hbar}S_c[x(t)]\}, \tag{2.47}$$

where $F(T)$ is the prefactor and $S_c[x(t)]$ is the classical action. The classical action can be calculated by the principle of least action. The classical equation of motion can be written in the form

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$$\ddot{x} + \omega^2 x = 0, \tag{2.48}$$

with conditions $x(t_1) = x_1, x(t_2) = x_2$, and the solution is

$$x(t) = A\sin[\omega(t+\alpha)], \tag{2.49}$$

where α is an initial phase. The action can be simplified by using the equation of motion in equation (2.48) and integration by parts. Using the equation of motion $\ddot{x} + \omega^2 x = 0$. We can write the action as

$$S_{cl} = \frac{m}{2}\left[x(t_2)\dot{x}(t_2) - x(t_1)\dot{x}(t_1)\right]. \tag{2.50}$$

Let us rewrite equation (2.49) in following form

$$\begin{aligned} x(t) &= A\sin\left[\omega(t-t_1) + \omega(t_1+\alpha)\right] \\ &= A\sin[\omega(t-t_1)]\cos[\omega(t_1+\alpha)] + A\sin[\omega(t_1+\alpha)]\cos[\omega(t-t_1)]. \end{aligned}$$

We can continue to write classical path

$$x(t) = \frac{1}{\omega}\dot{x}(t_1)\sin[\omega(t-t_1)] + x_1\cos[\omega(t-t_1)]. \tag{2.51}$$

For the particular condition value $t = t_2$, then we find

$$\dot{x}(t_1) = \frac{\omega}{\sin[\omega(t_2-t_1)]}\left\{x_2 - x_1\cos[\omega(t_2-t_1)]\right\}. \tag{2.52}$$

Similarly,

$$\dot{x}(t_2) = \frac{\omega}{\sin[\omega(t_2-t_1)]}\left\{-x_1 + x_2\cos[\omega(t_2-t_1)]\right\}. \tag{2.53}$$

The action in equation (2.50), we need the product

$$x(t_2)\dot{x}(t_2) = \frac{\omega}{\sin[\omega(t_2 - t_1)]}\left\{x_2^2\cos[\omega(t_2 - t_1)] - x_2x_1\right\},$$

$$x(t_1)\dot{x}(t_1) = \frac{\omega}{\sin[\omega(t_2 - t_1)]}\left\{-x_1^2\cos[\omega(t_2 - t_1)] + x_2x_1\right\}.$$

Using this result to calculate the action in equation (2.50) with $T = t_2 - t_1$. The classical harmonic oscillator action gives

$$S_c = \frac{m\omega}{2\sin\omega T}\left\{(x_2^2 + x_1^2)\cos\omega T - 2x_2x_1\right\}, \tag{2.54}$$

and the expression of Van-Vleck Pauli formula need for the prefactor,

$$\sqrt{-\frac{\partial^2 S_c}{\partial x_2 \partial x_1}} = \sqrt{\frac{m\omega}{2\sin\omega T}}. \tag{2.55}$$

Using equations (2.54) and (2.55), substituting into equation (2.47) to obtain the expression for the harmonic oscillator path integral,

$$K(x_2, T; x_1, 0) = \sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega T}}\exp\frac{i}{\hbar}\left\{\frac{m\omega}{2\sin\omega T}[(x_2^2 + x_1^2)\cos\omega T - 2x_2x_1]\right\}. \tag{2.56}$$

2.4.2 The Forced Harmonic Oscillator

The forced harmonic oscillator is an oscillator of the form acting on by a time-dependent external force $f(t)$, with the Lagrangian

$$L(x, \dot{x}) = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2x^2 + f(t)x. \tag{2.57}$$

Thus, the equation of motion is

$$\ddot{x}(t) + \omega^2 x(t) = \frac{f(t)}{m}, \tag{2.58}$$

and boundary conditions, $x(t_1) = x_1, x(t_2) = x_2$. We introduce the Green function to carry out the equation

$$\left[m\frac{d^2}{dt^2} + m\omega^2\right] G(t,s) = \delta(t-s), \tag{2.59}$$

with the Green function

$$\begin{aligned} G(t,s) &= -H(t-s)\frac{\sin\omega(s-t_1)\sin\omega(t_2-t)}{\omega\sin\omega(t_2-t_1)} \\ &= -H(s-t)\frac{\sin\omega(t-t_1)\sin\omega(t_2-s)}{\omega\sin\omega(t_2-t_1)} \end{aligned} \tag{2.60}$$

where $H(t,s)$ is a Heaviside step function. The classical path can be determined by considering equations (2.59) and (2.60). Using the boundary conditions of the classical path $x(t)$. We obtain

$$x(t) = \frac{x_2\sin\omega(t-t_1) + x_1\sin\omega(t_2-t)}{\sin\omega(t_2-t_1)} + \frac{1}{m}\int_{t_1}^{t_2} f(t)G(t,s)ds. \tag{2.61}$$

The classical action S_{cl} can be calculated by following the same procedure in equation (2.50), which is

$$S_{cl} = \frac{m}{2}\left[x_2\dot{x}(t_2) - x_1\dot{x}(t_1)\right] + \frac{1}{2}\int_{t_1}^{t_2} f(t)x(t)dt. \tag{2.62}$$

Therefore, the classical action of system can be determined as

$$\begin{aligned} S_{cl} = \frac{m\omega}{2\sin\omega(t_2-t_1)}\{(x_2^2+x_1^2)\cos\omega(t_2-t_1) - 2x_2x_1 + \frac{2x_2}{m\omega}\int_{t_1}^{t_2} dtf(t)\sin\omega(t_1-t) \\ + \frac{2x_1}{m\omega}\int_{t_1}^{t_2} dtf(t)\sin\omega(t_2-t) - \frac{2}{m^2\omega^2}\int_{t_1}^{t_2}\int_{t_1}^{t_2} dtdsf(t)f(s)\sin\omega(t_2-t)\sin\omega(s-t)\}. \end{aligned} \tag{2.63}$$

Finally, the Feynman propagator for an electron in a harmonic potential with the time dependent external force is

$$K(x_2, t_2; x_1, t_1) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin\omega(t_2 - t_1)}} \exp\{\frac{i}{\hbar} S_{cl}\}, \tag{2.64}$$

where the classical action can be defined in equation (2.63).

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Chapter 3
Review of Mathematical Models of Random Potential Systems

In this chapter, we review the mathematical model of random potential via the Feynman path integral formulation. The model is an electron coupling with a large system in the form of a random potential. In this model, we are interested in the approximate propagator which can be obtained by averaging the propagator over the coordinates of the large system.

3.1 Edwards' Model

The model of an electron moving in a completely random system containing dense and weak scatterers has been introduced by Edwards and Gulayev [4], Edwards [17], and Abram and Edwards [18].

3.1.1 Random Potential

The important problem in a disordered system is a model of an electron moving in a fluctuation potential or a random potential. The interaction between a free electron with a fluctuation potential caused by the imperfection of the system. The fluctuation potential [19] can be represented by the autocorrelation function $W \equiv \langle v(\vec{r}(t))v(\vec{r}(s))\rangle$ where $v(\vec{r}(t)), v(\vec{r}(s))$ are the time-dependent random potential and the angle brackets denote the ensemble average. The important characteristic parameters of the random potential are the magnitude of fluctuation energy (ξ) and the correlation length (l). There are two alternative

definitions of the fluctuation potential. Firstly, Anderson [20] discussed about an electron with a system of deep potential wells situated on given lattice points and separated by sufficiently high barriers. The second definition is from Lifshitz [21] who assumed that there are scatterers in the system. The scatterer being determined by its own field $v(\vec{r}-\vec{R}_i)$ which is called the scattering potential. In such cases, the random potential can be defined by the autocorrelation function which are dependent on the distance $|\vec{r}(t)-\vec{r}(s)|$ and the correlation length.

3.1.2 Action of the System

By considering a free electron moving in a set of N rigid scatterers confined within a volume V and a density $n = N/V$ and using the path integral method to derive the average Green function of the Schrödinger equation, the disordered system can be described by the Hamiltonian

$$H[v] = -\frac{\hbar^2}{2m}\nabla^2 + \sum_i v(\vec{r}-\vec{R}_i), \tag{3.1}$$

where $v(\vec{r}-\vec{R}_i)$ is the potential of single scatterer at site $\vec{R}_i$. The time-dependent Schrödinger equation for an electron of the effective mass m in disordered system is

$$(i\hbar\frac{\partial}{\partial t} - H[v])g(\vec{r}'\vec{r}, T0; [\vec{R}]) = \delta(\vec{r}' - \vec{r})\delta(t). \tag{3.2}$$

The Green function of the time-dependent Schrödinger equation can be expressed in the path integral representation as

$$g(\vec{r}'\vec{r}, T0; [\vec{R}]) = \int D[\vec{r}(t)] \exp\frac{i}{\hbar}\left\{\int_0^T dt[\frac{m}{2}\dot{\vec{r}}^2(t) - \sum_i v(\vec{r}(t)-\vec{R}_i)]\right\}, \tag{3.3}$$

where $D[\vec{r}(t)]$ denotes the path integral to be carried out with the boundary conditions $\vec{r}(0) = \vec{r}$ and $\vec{r}(T) = \vec{r}'$. The site $\vec{R}_i$ denotes that the scatterer is in random configuration $(\vec{R}_1, ..., \vec{R}_i, ...)$, specified by the probability distribution on configurations space,

$$P[\vec{R}]d[\vec{R}] = \frac{d\vec{R}_1, ..., d\vec{R}_N}{V^N} = \prod_{N,V\to\infty} \frac{d\vec{R}_i}{V}, \tag{3.4}$$

where V is a small volume on configurations space.

The propagator of random system $K(\vec{r}', T; \vec{r}, 0)$ is an ensemble average of the Green function with respect to the random scatterers configuration which is the integration of Green function with the probability distribution over all the configurations of the scatterers,

$$K(\vec{r}', T; \vec{r}, 0) = \left\langle g(\vec{r}'\vec{r}, T, 0; [\vec{R}]) \right\rangle_{[\vec{R}]} = \int g(\vec{r}'\vec{r}, T0; [\vec{R}]) P[\vec{R}]d[\vec{R}]$$

$$= \int \left\{ \exp \frac{i}{\hbar} \int_0^T [\frac{m}{2}\dot{\vec{r}}^2(t) - \sum_i v(\vec{r}(t) - \vec{R}_i)]dt \right\} D[\vec{r}(t)] \prod_{i=1}^{N} (\frac{d\vec{R}_i}{V})$$

$$= \int \exp\left\{ \frac{i}{\hbar} \int_0^T \frac{m}{2}\dot{\vec{r}}^2(t)dt \right\} \left\{ \int \exp[-\frac{i}{\hbar}\int_0^T v(\vec{r}(t) - \vec{R})dt \frac{d\vec{R}}{V}] \right\}^N D[\vec{r}(t)]. \tag{3.5}$$

By using the identity $e^x = (1+x/N)^N$ and the density of the scatterer is $n = N/V$. The propagator of random system [4] can be written as

$$K(\vec{r}', T; \vec{r}, 0) \equiv \left\langle g(\vec{r}'\vec{r}, T0; [\vec{R}]) \right\rangle_{[\vec{R}]} =$$

$$\int D[\vec{r}(t)] \exp \frac{i}{\hbar} \left\{ \int_0^T \frac{m}{2}\dot{\vec{r}}^2(t)dt + n \int d\vec{R} \left[\exp(-\frac{i}{\hbar}\int_0^T v(\vec{r} - \vec{R})dt) - 1 \right] \right\}. \tag{3.6}$$

This is the exact expression for a propagator or an average Green function.

For simplicity, we shall consider the limit of high density $n \to \infty$ and weak scatterer $v \to 0$ so that nv^2 remains finite. Since $\rho v^2 \gg \rho v^3$, the exponential can be expanded in the Taylor series. The average propagator can be written as

$$K(\vec{r}', T; \vec{r}, 0) = \int D[\vec{r}(t)] \exp\left\{ \frac{i}{\hbar} \int_0^T \frac{m}{2} \dot{\vec{r}}^2(t) dt - \frac{in}{\hbar} \int d\vec{R} \int_0^T v(\vec{r}(t) - \vec{R}) dt \right.$$

$$\left. - \frac{n}{2\hbar^2} \int d\vec{R} \int_0^T \int_0^T v(\vec{r}(t) - \vec{R}) v(\vec{r}(s) - \vec{R}) dt ds \right\}. \qquad (3.7)$$

The average potential energy density is defined as $E_0 = \langle v(\vec{r}(t)) \rangle = n \int d\vec{R} v(\vec{r}(t) - \vec{R})$. The autocorrelation function of scatterers $W(\vec{r}(t) - \vec{r}(s))$ is the effect of a potential at one point on a potential at another point that is the two points are correlated. The autocorrelation function can be defined as

$$W(\vec{r}(t) - \vec{r}(s)) \equiv \langle v(\vec{r}(t)) v(\vec{r}(s)) \rangle = \int d\vec{R} v(\vec{r}(t) - \vec{R}) v(\vec{r}(s) - \vec{R}). \qquad (3.8)$$

The expression of path integrals can be expressed formally in term of the action function S as

$$K(\vec{r}', T; \vec{r}, 0) = \int D[\vec{r}(t)] \exp\{ \frac{i}{\hbar} S \}, \qquad (3.9)$$

where the action S is defined by

$$S = \int_0^T dt \left[\frac{m}{2} \dot{\vec{r}}^2(t) - E_0 + \frac{in}{2\hbar} \int_0^T ds W(\vec{r}(t) - \vec{r}(s)) \right]. \qquad (3.10)$$

This action is sometimes called "two-time" action. The system can be viewed as an electron moving in the nonlocal potential with a memory effect. The autocorrelation function for a Gaussian random potential has the form

$$W(\vec{r}(t)-\vec{r}(s)) = \xi \cdot \exp\left(-\frac{|\vec{r}(t)-\vec{r}(s)|^2}{L^2}\right), \tag{3.11}$$

where the fluctuation energy ξ has the dimension of the energy squared and L is the Gaussian correlation length which can be defined by $L^2 = 2l^2$. In the limiting case of the Gaussian correlation length approaches to zero, the autocorrelation function approaches the delta function as

$$W(\vec{r}(t)-\vec{r}(s)) = D \cdot \delta(\vec{r}(t)-\vec{r}(s)), \tag{3.12}$$

where D is the magnitude of white noise energy. This is the white noise correlation function.

3.2 Path Integral Theory of an Electron Gas in a Random Potential : Bezak's Model

Bezak [7,22] proposed his model to describe the impurity band in a poly-crystalline semiconductor. The impurity can precipitate in the vicinity of interfaces between crystalline forming potential barrier, which is deep potential wells with the magnitude (η). This model represented the interaction as a random potential and the autocorrelation function as a Gaussian one. If the correlation length L is larger than the interatomic distance, we can approximate the Gaussian autocorrelation function by

$$W(\vec{r}(t)-\vec{r}(s)) = \exp\left(1-\frac{[\vec{r}(t)-\vec{r}(s)]^2}{L^2}\right), \tag{3.13}$$

and the propagator in equation (3.7) takes the form

$$K(\vec{r}^{\,\prime}, T; \vec{r}, 0) = \exp\left(-\frac{n\eta^2 T^2}{2\hbar^2}\right)$$

$$\times \int D[\vec{r}(t)] \exp \frac{i}{\hbar} \left\{ \int_0^T \frac{m}{2} \dot{\vec{r}}^2(t) dt - \frac{m\omega^2}{4T} \int_0^T \int_0^T dt ds [\vec{r}(t) - \vec{r}(s)]^2 \right\}, \tag{3.14}$$

where ω is the harmonic frequency related to the correlation length, l, by the relation $\omega^2 = 2in\eta^2 T/m\hbar l^2$. The action of Bezak's model can be defined with the one-parameter nonlocal harmonic random potential as

$$S(\omega) = \int_0^T \frac{m}{2} \dot{\vec{r}}^2(t) dt - \frac{m\omega^2}{4T} \int_0^T \int_0^T dt ds (\vec{r}(t) - \vec{r}(s))^2. \tag{3.15}$$

The propagator of an electron moving in a random potential has been calculated by Bezak [7], and Khandekar and Lawande [23], as

$$K(\vec{r}', T; \vec{r}, 0) = (\frac{m}{2\pi i\hbar T})^{3/2} (\frac{\omega T}{2 \sin \omega T})^3 \exp \frac{i}{\hbar} \left\{ \frac{m\omega}{4} \cot(\frac{\omega T}{2}) (\vec{r}' - \vec{r})^2 - \frac{in\eta^2 T^2}{2\hbar} \right\}. \tag{3.16}$$

3.3 Two-Particle Model System

In this section, we present the model used by Samathiyakanit [8] and use his trial action which contains two parameters, $S(\kappa, \omega)$. The impurity in a random system produces the random potential interacting with an electron. The effect of the impurity field is produced by the fictitious particle of mass M. Physically, this model is a free electron interacts harmonically with a fictitious particle of mass M with κ as a spring constant and the harmonic frequency is $\omega = \sqrt{\kappa/M}$. The The Lagrangian of two-particle model system can be written as

$$L = \frac{1}{2} m \dot{\vec{X}}^2(t) + \frac{1}{2} M \dot{\vec{Y}}^2(t) - \frac{1}{2} \kappa (\vec{X}(t) - \vec{Y}(t))^2, \tag{3.17}$$

where M and $\vec{Y}$ are the mass and the coordinate of fictitious particle, respectively. Then the path integral of this Lagrangian can be written as

$$K\left(\vec{X}_2, \vec{Y}_2, T; \vec{X}_1, \vec{Y}_1, 0\right) = \int D[\vec{X}(t)]D[\vec{Y}(t)] \exp\left[\int_0^T dt L(\vec{X}, \vec{Y}, t)\right]. \quad (3.18)$$

The coordinate of the fictitious particles can be eliminated by setting $\vec{Y}_2 = \vec{Y}_1$. Integrating the propagator of two-particle system over the coordinate $\vec{Y}_2$ (see Appendix for more details) yields the average effect of the fictitious particles on the electron. Therefore, the action of the two-particle model system has only the electron coordinate, which is

$$S(\omega, \kappa) = \int_0^T dt \frac{1}{2} m\dot{\vec{r}}^2(t) - \frac{\kappa\omega}{8} \int_0^T \int_0^T dt ds (\vec{r}(t) - \vec{r}(s))^2 \frac{\cos\omega(\frac{T}{2} - |t-s|)}{\sin\frac{\omega}{2}T}. \quad (3.19)$$

In fact, this action can be reduced to the action of Bezak's model by setting $\omega \to 0$ or equivalently $M \to \infty$.

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Chapter 4
Results

This chapter, we will calculate the exact two-dimensional propagator in the transverse magnetic field and the x-directional electric field with a two-parameter nonlocal harmonic potential. In this calculation we introduce the two-parameter nonlocal harmonic random potential [8] to describe the potential of our system.

4.1 Two-Dimensional Propagators

We consider the non-interacting electron gas in the two-dimensional random system. The model of interest involves an electron moving in a two-dimensional random system with a transverse magnetic field and an x-directional electric field. The impurity in a random system produces the random potential interacting with an electron. Thus, the Lagrangian of the system is

$$L(x,y) = \frac{m}{2}\left[\dot{\vec{x}}^2(t) + \dot{\vec{y}}^2(t)\right] + \frac{\Omega}{2}[x(t)\dot{y}(t) - y(t)\dot{x}(t)]$$
$$-\frac{\kappa\omega}{8}\int_0^T ds \frac{\cos\omega(T/2-|t-s|)}{\sin\omega(T/2)}\left[(\vec{x}(t)-\vec{x}(s))^2 + (\vec{y}(t)-\vec{y}(s))^2\right]$$
$$+e\vec{E}_x(t)\cdot\vec{x}(t), \tag{4.1}$$

where $\Omega = eB/mc$ is the cyclotron frequency and a symmetric gauge of a magnetic field $\vec{B}_z$ with the vector potential, $\vec{A} = (1/2)(yB, -xB, 0)$. The Lagrangian describes an electron moving in a two-dimensional system under the influence of a nonlocal harmonic random potential with a transverse magnetic and an

x-direction electric fields. We see that the Lagrangian of system is a two-time quadratic form. From §2.3.2, the propagator can be expressed by the contribution of the classical action. Therefore, we will evaluate the classical action and the prefactor of system.

4.1.1 The Classical Action

From the principle of least action, we cannot calculate the classical action exactly because an equation of motion is the set of coupled integro-differential equation due to a symmetric gauge. However, a classical action can be calculated by applying the two-particle method [8] and the first-order cumulant approximation [24]. The two-dimensional propagator can be expressed by a product of the x-component propagator and the y-component propagator as

$$K(x_T, y_T, T; x_0, y_0, 0) = K_x(x_T, T; x_0, 0) K_y(y_T, T; y_0, 0), \tag{4.2}$$

with Lagrangians of the system are

$$\begin{aligned} L_x = \frac{m}{2}\dot{\vec{x}}^2(t) + \frac{\Omega}{2}(x(t)\dot{y}(t) - y(t)\dot{x}(t)) + e\vec{E}_x(t)\cdot\vec{x}(t) \\ -\frac{1}{8}\kappa\omega\int_0^T ds \frac{\cos\omega(T/2 - |t-s|)}{\sin\omega(T/2)}(\vec{x}(t) - \vec{x}(s))^2, \end{aligned} \tag{4.3}$$

and

$$L_y = \frac{m}{2}\dot{\vec{y}}^2(t) - \frac{1}{8}\kappa\omega\int_0^T ds \frac{\cos\omega(T/2 - |t-s|)}{\sin\omega(T/2)}(\vec{y}(t) - \vec{y}(s))^2. \tag{4.4}$$

Firstly, we consider the x-component propagator and integrate by parts the magnetic field term

$$\int_0^T (x\dot{y} - y\dot{x})dt = -(x_T y_T - x_0 y_0) + 2\int_0^T x\dot{y}dt. \tag{4.5}$$

Let us carry out the x-component propagator of the Lagrangian in equation (4.3) by using equation (4.5). The x-component propagator can be written in the form

$$K_x(x_T, x_0; T) = \exp\left(-\frac{i\Omega}{2\hbar}[x_T y_T - x_0 y_0]\right) \int D[\vec{x}(t)] \exp\frac{i}{\hbar}\int_0^T dt \left\{\frac{m}{2}\dot{\vec{x}}^2(t) \right.$$
$$\left. -\frac{1}{8}\kappa\omega\int_0^T ds \frac{\cos\omega(T/2 - |t-s|)}{\sin\omega(T/2)}(\vec{x}(t) - \vec{x}(s))^2 + \vec{f}(t)\cdot\vec{x}(t)\right\}, \tag{4.6}$$

where the external force can be defined as

$$f(t) = [\Omega\dot{y}(t) + eE_x(t)]\,. \tag{4.7}$$

Referring to §3.3, we applied the two-particle model system. This propagator can be calculated by the two-particle system. The two-particle system is described by an electron of mass m coupling with an another particle of mass M with a force constant κ. We obtain the classical path in three dimensions from the Lagrangian in equation (3.16) as

$$L = \frac{1}{2}\left[m\dot{\vec{X}}^2(t) + M\dot{\vec{Y}}^2(t) - \kappa(\vec{X}(t) - \vec{Y}(t))^2\right] + \vec{f}(t)\cdot\vec{X}(t). \tag{4.8}$$

It is obviously seen that the equation of motion is a set of coupled equations. Such a problem can be solved by transforming the Lagrangian into the center of mass coordinate system

$$\vec{r} = \vec{X} - \vec{Y}, \vec{R} = \frac{m\vec{X} + M\vec{Y}}{m+M}$$
$$m_0 = m + M, \mu = \frac{mM}{m+M}, \tag{4.9}$$

where $\vec{r}$ is a relative coordinate and $\vec{R}$ is a center of mass coordinate. Hence, the Lagrangian can be written as containing two coupled systems with a forced harmonic oscillator

$$L = \frac{1}{2}(\mu\dot{\vec{x}}^2 - \kappa\vec{x}^2) + \frac{\mu}{m}\vec{f}\cdot\vec{x} + \frac{1}{2}m_0\dot{\vec{R}}^2 + \vec{f}\cdot\vec{R}, \tag{4.10}$$

where m_0 and μ are the total mass and the reduced mass, respectively. This can be interpreted that there are two non-interacting forced harmonic oscillators which one of mass μ has a frequency $\nu = \sqrt{\kappa/\mu}$ and is acted by the force $\mu\vec{f}/m$, but the other has mass m_0, no frequency, and is acted by the force $\vec{f}$. From the two-particle model system, the classical action can be calculated exactly by Samathiyakanit [8] as

$$\begin{aligned}
S_{cl}^f = &\left(\frac{\mu\nu}{4}\cot\frac{\nu}{2}T + \frac{1}{2}\frac{m\mu}{MT}\right)(\vec{r}_T - \vec{r}_0)^2 \\
&+\vec{r}_T\cdot\int_0^T dt\vec{f}(t)\left(\frac{\mu}{m}(\frac{\sin\nu t}{\sin\nu T} - \frac{\sin\frac{\nu}{2}(T-t)\sin\frac{\nu}{2}t}{\cos\frac{\nu}{2}T}) + \frac{\mu t}{MT}\right) \\
&+\vec{r}_0\cdot\int_0^T dt\vec{f}(t)\left(\frac{\mu}{m}(\frac{\sin\nu(T-t)}{\sin\nu T} - \frac{\sin\frac{\nu}{2}(T-t)\sin\frac{\nu}{2}t}{\cos\frac{\nu}{2}T}) + \frac{\mu(T-t)}{MT}\right) \\
&-\int_0^T\int_0^T dtds\vec{f}(t)\cdot\vec{f}(s)\left(\frac{\mu^2}{m^2}(\frac{\sin\nu(T-t)\sin\nu s}{\nu\sin\nu T}\right. \\
&\left.-\frac{4\sin\frac{\nu}{2}(T-t)\sin\frac{\nu}{2}t\sin\frac{\nu}{2}(T-s)\sin\frac{\nu}{2}s}{\nu\sin\nu T}) + \frac{\mu(T-t)s}{MT}\right).
\end{aligned} \tag{4.11}$$

Applying the classical action of the two-particle system in equation (4.11), and substituting the notation of external force in equation (4.7), then we obtain the x-component propagator

$$K_x(x_T, x_0; T) = F(T)\exp\frac{i}{\hbar}\left\{S_{x,Cl}^0 - \frac{\Omega}{2}(x_T y_T - x_0 y_0)\right.$$

$$+x_T\int_0^T dt[\Omega\dot{y}(t)+eE_x(t)]g_1(t)+x_0\int_0^T dt[\Omega\dot{y}(t)+eE_x(t)]g_2(t)$$

$$-\int_0^T\int_0^T dtds[\Omega\dot{y}(t)+eE_x(t)][\Omega\dot{y}(s)+eE_x(s)]G(t,s)\Big\}, \qquad (4.12)$$

where

$$S^0_{x,Cl}=(\frac{\mu\nu}{4}\cot\frac{\nu}{2}T+\frac{1}{2}\frac{m\mu}{MT})(x_T-x_0)^2, \qquad (4.13)$$

$$g_1(t)=\frac{\mu}{m}(\frac{\sin\nu t}{\sin\nu T}-\frac{\sin\frac{\nu}{2}(T-t)\sin\frac{\nu}{2}t}{\cos\frac{\nu}{2}T})+\frac{\mu t}{MT}, \qquad (4.14)$$

$$g_2(t)=\frac{\mu}{m}(\frac{\sin\nu(T-t)}{\sin\nu T}-\frac{\sin\frac{\nu}{2}(T-t)\sin\frac{\nu}{2}t}{\cos\frac{\nu}{2}T})+\frac{\mu(T-t)}{MT}, \qquad (4.15)$$

$$G(t,s)=\frac{\mu^2}{m^2}(\frac{\sin\nu(T-t)\sin\nu s}{\nu\sin\nu T}$$

$$-\frac{4\sin\frac{\nu}{2}(T-t)\sin\frac{\nu}{2}t\sin\frac{\nu}{2}(T-s)\sin\frac{\nu}{2}s}{\nu\sin\nu T})+\frac{\mu(T-t)s}{MT}. \qquad (4.16)$$

In addition, the classical action is separated into two parts, which are the classical forced nonlocal harmonic action in the x-component and the time derivative of the y-component. The integral of a time derivative of the y-component can be carried out by integration by parts term by term. Therefore, the x-component propagator can be rewritten as

$$K_x(x_T,x_0;T)=F(T)\exp\frac{i}{\hbar}\Big\{S^f_{x,Cl}+S'[y(t)]+\Omega\frac{4\mu-m}{2m}x_Ty_T+\Omega\frac{4\mu+m}{2m}x_0y_0$$

$$-2y_T\Omega\int_0^T dteE_x(t)(\frac{\mu\sin\nu(T-t)}{m^2\nu}+\frac{\mu(T-t)}{mM})\Big\}, \qquad (4.17)$$

where the action

$$
\begin{aligned}
S^f_{x,Cl} = &\left(\frac{\mu\nu}{4}\cot\frac{\nu}{2}T + \frac{1}{2}\frac{m\mu}{MT}\right)(x_T - x_0)^2 \\
&+x_T\int_0^T dteE_x(t)\left(\frac{\mu}{m}(\frac{\sin\nu t}{\sin\nu T} - \frac{\sin\frac{\nu}{2}(T-t)\sin\frac{\nu}{2}t}{\cos\frac{\nu}{2}T}) + \frac{\mu t}{MT}\right) \\
&+x_0\int_0^T dteE_x(t)\left(\frac{\mu}{m}(\frac{\sin\nu(T-t)}{\sin\nu T} - \frac{\sin\frac{\nu}{2}(T-t)\sin\frac{\nu}{2}t}{\cos\frac{\nu}{2}T}) + \frac{\mu(T-t)}{MT}\right) \\
&-e^2\int_0^T\int_0^T dtdsE_x(t)E_x(s)\left(\frac{\mu^2}{m^2}(\frac{\sin\nu(T-t)\sin\nu s}{\nu\sin\nu T}\right. \\
&\left.-\frac{4\sin\frac{\nu}{2}(T-t)\sin\frac{\nu}{2}t\sin\frac{\nu}{2}(T-s)\sin\frac{\nu}{2}s}{\nu\sin\nu T}) + \frac{\mu(T-t)s}{MT}\right), \qquad (4.18)
\end{aligned}
$$

and

$$
\begin{aligned}
S^{'}[y(t)] = &-(x_T + x_0)\Omega\int_0^T dty(t)(\frac{\mu\nu\cos\frac{\nu}{2}(T-2t)}{2m\sin\frac{\nu}{2}T} + \frac{\mu}{mT}) \\
&+2\Omega\int_0^T dteE_x(t)\frac{\mu\sin\frac{\nu}{2}(T-t)}{m^2\sin\frac{\nu}{2}T}\int_0^T dsy(s)\cos\frac{\nu}{2}(t-2s) \\
&+2\Omega\int_0^T dteE_x(t)\frac{\mu(T-t)}{mMT}\int_0^T dsy(s) \\
&+\Omega^2\int_0^T\int_0^T dtdsy(t)y(s)(\frac{\mu\nu}{2m^2}\frac{\cos\nu(\frac{T}{2}-(t-s))}{\sin\frac{\nu}{2}T} + \frac{\mu}{mMT}).
\end{aligned} \qquad (4.19)
$$

Secondly, we will calculate the y-component propagator. By applying an action, $S^{'}[y(t)]$, in equation (4.19), we combine this action with the trial action, $S_0[y(t)]$, of a y-component Lagrangian in equation (4.4) and inserting the identity of trial action. The y-component propagator can be written as

$$
K_y(y_T, T; y_0, 0) = \frac{\int D[y(t)]\exp\frac{i}{\hbar}\left\{S_0[y(t)] + S^{'}[y(t)] + S_0[y(t)]\right\}}{\int D[y(t)]\exp\frac{i}{\hbar}\left\{S_0[y(t)]\right\}}. \qquad (4.20)
$$

Since an average is defined by

$$\langle f[y(t)]\rangle_{S_0} = \frac{\int D[y(t)] f[y(t)] \exp\{\frac{i}{\hbar} S_0[y(t)]\}}{\int D[y(t)] \exp\{\frac{i}{\hbar} S_0[y(t)]\}}. \tag{4.21}$$

The cumulant approximation [24] is

$$\left\langle \exp[\frac{i}{\hbar} S] \right\rangle_{S_0} = \exp\left\{ \frac{i}{\hbar}\langle S\rangle_{S_0} + (\frac{i}{\hbar})^2 \frac{1}{2}\left(\langle S^2\rangle_{S_0} - \langle S\rangle^2_{S_0}\right) + ... \right\}, \tag{4.22}$$

and keeping only the first-order term, which is the first-order cumulant approximation, $\left\langle e^{ix/\hbar} \right\rangle \sim e^{i\langle x\rangle/\hbar}$. Then the exponential in equation (4.20) can be separated to the exponential of a trial action and the average of action, $\langle S' \rangle_{S_{y,0}}$. The y-component propagator is contributed by a classical path as

$$K_y(y_T, T; y_0, 0) = K_{y,0}(y_T, T; y_0, 0) \exp \frac{i}{\hbar} \langle S' \rangle_{S_0}, \tag{4.23}$$

where the trial propagator

$$K_{y,0}(y_T, T; y_0, 0) = \exp \frac{i}{\hbar} \left(\frac{\mu\nu}{4} \cot \frac{\nu}{2} T + \frac{1}{2} \frac{m\mu}{MT} \right) (y_T - y_0)^2, \tag{4.24}$$

and

$$\begin{aligned}
\langle S' \rangle_{S_0} = & -(x_T + x_0)\Omega \int_0^T dt \langle y(t)\rangle_{S_0} \left(\frac{\mu\nu \cos\frac{\nu}{2}(T-2t)}{2m \sin\frac{\nu}{2}T} + \frac{\mu}{mT} \right) \\
& + 2\Omega \int_0^T dt e E_x(t) \frac{\mu \sin\frac{\nu}{2}(T-t)}{m^2 \sin\frac{\nu}{2}T} \int_0^T ds \langle y(s)\rangle_{S_0} \cos\frac{\nu}{2}(t-2s) \\
& + 2\Omega \int_0^T dt e E_x(t) \frac{\mu(T-t)}{mMT} \int_0^T ds \langle y(s)\rangle_{S_0} \\
& + \Omega^2 \int_0^T \int_0^T dt ds \langle y(t) y(s)\rangle_{S_0} \left(\frac{\mu\nu}{2m^2} \frac{\cos\nu(\frac{T}{2} - (t-s))}{\sin\frac{\nu}{2}T} + \frac{\mu}{mMT} \right).
\end{aligned} \tag{4.25}$$

We see that equation (4.25) contains the average over quantities like $\langle y(t)\rangle_{S_0}$ and $\langle y(t)y(s)\rangle_{S_0}$. These quantities can be evaluated from the generating function [25]. The generating function is defined as

$$\left\langle \exp\left[\int_0^T dt\vec{f}(t)\cdot\vec{r}(t)\right]\right\rangle_{S_0} = \frac{\int D[\vec{r}(t)]\exp[S_0+\int_0^T dt\vec{f}(t)\cdot\vec{r}(t)]}{\int D[\vec{r}(t)]\exp[S_0]}, \tag{4.26}$$

with end points condition $\vec{r}(T)=\vec{r}_T, \vec{r}(0)=\vec{r}_0$ and $\vec{f}(t)$ is a time-dependent arbitrary function. From Feynman and Hibbs [25], we are thus left with is the exponential of the two classical action, that is

$$\left\langle \exp\left[\int_0^T dt\vec{f}(t)\cdot\vec{r}(t)\right]\right\rangle_{S_0} = \exp\left(S_{cl}^f - S_{cl}^0\right). \tag{4.27}$$

Hence, we can see that the quantities of interest can be extracted from the formula in equation (4.27) by performing the functional differentiation with respect to the function $\vec{f}(t)$ and setting it to be zero. For examples,

$$\begin{aligned}\left\langle \vec{r}(t)\exp\left[\int_0^T dt\vec{f}(t)\cdot\vec{r}(t)\right]\right\rangle_{S_0} &= \frac{\delta}{\delta\vec{f}(t)}[\exp(S_{cl}^f - S_{cl}^0)] \\ &= \frac{\delta S_f}{\delta\vec{f}(t)}[\exp(S_{cl}^f - S_{cl}^0)].\end{aligned} \tag{4.28}$$

Therefore, by evaluating both sides when $\vec{f}(t)\equiv 0$, we obtain

$$\langle\vec{r}(t)\rangle_{S_0} = \left[\frac{\delta S_{cl}^f}{\delta\vec{f}(t)}\right]_{\vec{f}\equiv 0}. \tag{4.29}$$

We can continue this process to get the second derivatives as

$$\begin{aligned}\langle\vec{r}(t)\cdot\vec{r}(s)\rangle_{S_0} &= \frac{\delta^2}{\delta\vec{f}(t)\delta\vec{f}(s)}\exp(S_{cl}^f - S_{cl}^0)\mid_{\vec{f}\equiv 0} \\ &= \left[\frac{\hbar}{i}\frac{\delta^2 S_{cl}^f}{\delta\vec{f}(t)\delta\vec{f}(s)} + \frac{\delta S_{cl}^f}{\delta\vec{f}(t)}\frac{\delta S_{cl}^f}{\delta\vec{f}(s)}\right]_{\vec{f}\equiv 0}.\end{aligned} \tag{4.30}$$

Actually, since S_{cl}^f is quadratic in $\vec{f}(t)$, the quantities $\langle\vec{r}(t)\rangle_{S_0}$ and $\langle\vec{r}(t)\cdot\vec{r}(s)\rangle_{S_0}$ can be directly evaluated in terms of $\delta S_{cl}^f/\delta\vec{f}(t)$ and $\delta^2 S_{cl}^f/\delta\vec{f}(t)\delta\vec{f}(s)$, which is independent of $\vec{f}(t)$.

Next, by applying the generating functional technique, we can evaluate the quantities $\langle y(t)\rangle_{S_0}$ and $\langle y(t)y(s)\rangle_{S_0}$ in equation (4.25). First, we will evaluate these quantities by introducing the Lagrangian of forced nonlocal harmonic as

$$L_y = \frac{m}{2}\dot{\vec{y}}^2(t) - \frac{\kappa\omega}{8}\int_0^T ds\frac{\cos(\frac{T}{2}-|t-s|)}{\sin(\omega T/2)}(\vec{y}(t)-\vec{y}(s))^2 + \vec{f}(t)\cdot\vec{y}(t), \tag{4.31}$$

and the classical action S_f can be evaluated in the equation (4.11). Substituting S_f in equation (4.11) of the y-component into equations (4.29) and (4.30), we obtain

$$\begin{aligned}\langle y(t)\rangle_{S_0} = y_T&\left(\frac{\mu}{m}\frac{\cos\frac{\nu}{2}(T-t)\sin\frac{\nu}{2}t}{\sin\frac{\nu}{2}T}+\frac{\mu t}{MT}\right)\\ &+y_0\left(\frac{\mu}{m}\frac{\sin\frac{\nu}{2}(T-t)\cos\frac{\nu}{2}t}{\sin\frac{\nu}{2}T}+\frac{\mu(T-t)}{MT}\right)\end{aligned} \tag{4.32}$$

and

$$\begin{aligned}\langle y(t)y(s)\rangle_{S_0} = &\left(\frac{2\mu}{m^2\nu}\frac{\sin\frac{\nu}{2}(T-t)\sin\frac{\nu}{2}s\cos\frac{\nu}{2}(T-t)}{\sin\frac{\nu}{2}T}+\frac{\mu(T-t)s}{mMT}\right)\\ &+\left(y_0\left[\frac{\mu}{m}\frac{\sin\frac{\nu}{2}(T-t)\cos\frac{\nu}{2}t}{\sin\frac{\nu}{2}T}+\frac{\mu(T-t)}{MT}\right]\right.\\ &\left.+y_T\left[\frac{\mu}{m}\frac{\cos\frac{\nu}{2}(T-t)\sin\frac{\nu}{2}t}{\sin\frac{\nu}{2}T}+\frac{\mu t}{MT}\right]\right)^2.\end{aligned} \tag{4.33}$$

Substituting equations (4.32) and (4.33) into equation (4.25), we can be evaluated $\langle S'\rangle_{S_0}$ by integrating term by term. Then an average of the action, $\langle S'\rangle_{S_0}$, can be rewritten as

$$\langle S^{'}\rangle_{S_0} = -\Omega^2\left\{A(t)+B(t)\right\} - \Omega\{(\frac{\mu^2}{m^2\nu}+\frac{\mu^2}{m^2})(x_T+x_0)(y_T+y_0)\}$$

$$-2\Omega\int_0^T dteE_x(t)\{y_T G_1(t)+y_0 G_2(t)\} \tag{4.34}$$

where

$$G_1(t) = \frac{\nu}{8m^3\nu\sin\frac{\nu}{2}T}\Big(2\nu T\sin^2\frac{\nu}{2}(T-t)+3\sin\frac{\nu}{2}(T-t)\cos\frac{\nu}{2}(3T-t)$$

$$-2\sin\nu(T-t)+\sin\frac{\nu}{2}(T-t)\cos\frac{\nu}{2}(T+t)\Big),$$

$$G_2(t) = \frac{\nu}{8m^3\nu\sin\frac{\nu}{2}T}\Big(-2\nu T\sin^2\frac{\nu}{2}(T-t)+3\sin\frac{\nu}{2}(T-t)\cos\frac{\nu}{2}(T+t)$$

$$-2\sin\nu(T-t)+\sin\frac{\nu}{2}(T-t)\cos\frac{\nu}{2}(3T-t)\Big),$$

$$A(T) = \frac{\mu^2}{32m^4M^2T\nu^3\sin^2\frac{\nu}{2}T}\Big(\nu T\Big[16mM+4(m^2-M^2)\nu^2T^2$$

$$-(M^2+4m^2\nu^2T^2)\cos\nu T-16mM\cos 2\nu T+M^3\cos 3\nu T\Big]$$

$$+8M\sin\nu T\Big[-4m+M^2\nu^2T^2+(4m-2m\nu^2T^2)\cos\nu T.\Big]\Big),$$

$$B(T) = \frac{\mu^3}{24m^4M^3T^2\nu^3}$$

$$\times\Big\{\Big[6mM\nu(8m+3MT)+2T^2\nu^3(m(4m^2+6mM+3M^2)-3M^2T(3m+M))$$

$$+3mMT\nu((16m-10M)\cos\nu T-\nu((8m+2M-2MT)\cot\frac{\nu}{2}T-MT\nu\csc^2\frac{\omega}{2}T)$$

$$+2M(-24m^2+\nu^2T^2(12M^2+18mM+7M^2))\sin\nu T\Big]y_0^2$$

$$+2m\nu\Big[(-6M(MT+8m+4mT)+\nu^2T^2(4m^2+12mM+3M^2)-6MT(4m+M)$$
$$\cos\nu T-3MT\nu((8m+2M+2MT)\cot\frac{\nu}{2}T+MT\nu\csc^2\frac{\omega}{2}T)$$
$$+2M(24m^2+MT^2\nu^2(3m+2M))\Big]y_0y_T$$

$$+\frac{\nu}{MT^2}\Big[(6mM(5M^3T^3+8m(M^2T^2+M^2T^3))+2MT^3\nu^2(4m^3MT+6m^2M^2T$$
$$+3M^3T^2+3mM^2(MT+MT^2))-3mM^2T^2(6M^2T\cos\nu T$$
$$+2\nu(4mMT+M^2(T+T^2)\cot\frac{\nu}{2}T)-M^2T^2\nu^2\csc^2\frac{\nu}{2}T))$$
$$+2M(24m^2+MT^2\nu^2(3m+2M))\sin\nu T\Big]y_T^2\Big\}. \qquad (4.35)$$

Finally, the full classical action is a product of the classical action of the x-component in equation (4.17) and the classical action of the y-component in equation (4.33), which is

$$S_{cl}[x,y]=\exp\Big\{S^0_{cl,x,y}-\Omega^2[A(T)+B(T)]+\Omega\frac{4\mu-m}{2m}x_Ty_T+\Omega\frac{4\mu+m}{2m}x_0y_0$$
$$-\Omega((\frac{\mu^2}{m^2\nu}+\frac{\mu^2}{m^2})(x_T+x_0)(y_T+y_0))$$
$$-2\Omega\int_0^T dteE_x(t)(y_TG_1(t)+y_0G_2(t))$$
$$-2y_T\Omega\int_0^T dteE_x(t)(\frac{\mu\sin\nu(T-t)}{m^2\nu}+\frac{\mu(T-t)}{mM})$$
$$+x_T\int_0^T dteE_x(t)(\frac{\mu}{m}[\frac{\sin\nu t}{\sin\nu T}-\frac{\sin\frac{\nu}{2}(T-t)\sin\frac{\nu}{2}t}{\cos\frac{\nu}{2}T}]+\frac{\mu t}{MT})$$
$$+x_0\int_0^T dteE_x(t)(\frac{\mu}{m}[\frac{\sin\nu(T-t)}{\sin\nu T}-\frac{\sin\frac{\nu}{2}(T-t)\sin\frac{\nu}{2}t}{\cos\frac{\nu}{2}T}]+\frac{\mu(T-t)}{MT})$$
$$-e^2\int_0^T\int_0^T dtdsE_x(t)E_x(s)(\frac{\mu^2}{m^2}[\frac{\sin\nu(T-t)\sin\nu s}{\nu\sin\nu T}$$
$$-\frac{4\sin\frac{\nu}{2}(T-t)\sin\frac{\nu}{2}t\sin\frac{\nu}{2}(T-s)\sin\frac{\nu}{2}s}{\nu\sin\nu T}]+\frac{\mu(T-t)s}{MT})\Big\}. \qquad (4.36)$$

4.1.2 The Prefactor

From the Feynman propagator, we will calculate the prefactor $F(T)$. An explicit expression for this function may be given from the classical solution by introducing a generating functional [26].

According to equation (2.45), we differentiate both sides by the operator $\kappa\partial/\partial\kappa$ and using notation of the average in equation (4.21). We obtain

$$-i\hbar\kappa\frac{\partial}{\partial\kappa}\ln F(T) = \left\langle \kappa\frac{\partial S_{F=0}}{\partial\kappa}\right\rangle_{S_0}. \tag{4.37}$$

We substitute an action of the Lagrangian in equation (4.1) into an above equation, neglecting magnetic and electric fields, becomes

$$-i\hbar\kappa\frac{\partial}{\partial\kappa}\ln F(T) = -\frac{1}{8}\kappa\omega\int_0^T\int_0^T dtds\frac{\cos\omega(\frac{T}{2}-|t-s|)}{\sin\frac{\omega}{2}T}\left\langle[\vec{r}(t)-\vec{r}(t)]^2\right\rangle_{S=0}, \tag{4.38}$$

where we define $\vec{r}(t)$ as a two-dimensional coordinate.

Next, we can calculate the average $\langle[\vec{r}(t)-\vec{r}(t)]^2\rangle_{S=0}$ by introducing the generating functional. We expand an average as $\langle\vec{r}^2(t)\rangle_{S_0} - 2\langle\vec{r}(t)\cdot\vec{r}(s)\rangle_{S_0} + \langle\vec{r}^2(s)\rangle_{S_0}$. From the previous section an average $\langle[\vec{r}(t)-\vec{r}(t)]^2\rangle_{S_0}$ becomes

$$\left\langle[\vec{r}(t)-\vec{r}(t)]^2\right\rangle_{S_0} = \frac{\mu^2}{m^2}\left[\frac{\sin\frac{\nu}{2}(t-s)\cos\frac{\nu}{2}(T-(t+s))}{\sin\frac{\nu}{2}T}+\frac{m(t-s)}{MT}\right]^2(\vec{r}_T-\vec{r}_0)^2$$

$$-2i\hbar\frac{\mu}{m}\left[\frac{2\sin\frac{\nu}{2}(t-s)\sin\frac{\nu}{2}(T-(t-s))}{m\nu\sin\frac{\nu}{2}T}+\frac{(t-s)(T-(t-s))}{MT}\right]. \tag{4.39}$$

Although, the prefactor is independent with the end points. We can set the limit of the end points condition by $\vec{r}(T) = \vec{r}(0) = 0$. Neglecting the first term on

the right hand side in equation (4.39) and substituting into equation (4.38), we obtain

$$-i\hbar\kappa\frac{\partial}{\partial\kappa}\ln F(T) = -\frac{\kappa\omega}{4}\left\{\frac{2i\hbar\mu}{m}[-\frac{2}{m\nu}\frac{\nu T}{2\omega(\nu^2-\omega^2)}(\nu\cot\frac{\nu}{2}T-\omega\cot\frac{\omega}{2}T)\right.$$
$$\left.+\frac{2}{M\omega^3}-\frac{T}{M\omega^2}\cot\frac{\omega}{2}T]\right\}. \tag{4.40}$$

Since, $\nu=\sqrt{\kappa/\mu}$ and $\omega=\sqrt{\kappa/M}$ are the relative (center of mass) harmonic and harmonic frequency respectively, harmonic frequencies and the force constant κ are related by

$$\frac{\kappa}{m}=\nu^2-\omega^2. \tag{4.41}$$

We can rewrite equation (4.40) as

$$-i\hbar\kappa\frac{\partial}{\partial\kappa}\ln F(T) = i\hbar\frac{\kappa T}{2m\nu}\left(\cot\frac{\nu}{2}T-\frac{2}{\nu T}\right). \tag{4.42}$$

According to equation (4.42), we can carry out the prefactor by introducing the expression

$$\frac{\partial\nu}{\partial\kappa}=\frac{1}{2m\nu},$$

and substitute into equation (4.42), to obtain

$$\frac{\partial}{\partial\nu}\ln F(T) = 2\left(\frac{1}{\nu}-\frac{1}{2}T\cot\frac{\nu}{2}T\right). \tag{4.43}$$

Integrating both sides of equation (4.43), we obtain the prefactor for the particle in random potential,

$$F(T) = C(t)\left(\frac{\nu}{\sin\frac{\nu}{2}T}\right)^2. \tag{4.44}$$

Comparing equation (4.44) with a prefactor for a free particle ($\kappa = 0, \nu = \omega$), we have

$$\frac{m}{2\pi i\hbar T} = C(t)\left(\frac{\omega}{\sin\frac{\omega}{2}T}\right)^2. \tag{4.45}$$

Finally, the full prefactor can be written as

$$F(T,\omega,\nu) = \frac{m}{2\pi i\hbar T}\left(\frac{\nu\sin\frac{\omega}{2}T}{\omega\sin\frac{\nu}{2}T}\right)^2. \tag{4.46}$$

4.1.3 Two-dimensional propagators

The analytic two-dimensional propagator in x-direction electric and magnetic fields with a two-parameter nonlocal harmonic potential is

$$\begin{aligned}
K(x_T,y_T,T;x_0,y_0,0) &= \frac{m}{2\pi i\hbar T}\left(\frac{\nu\sin\frac{\omega}{2}T}{\omega\sin\frac{\nu}{2}T}\right)^2 \\
&\cdot\exp\frac{i}{\hbar}\Big\{S^0_{cl,x,y} - \Omega^2[A(T)+B(T)] + \Omega\frac{4\mu-m}{2m}x_Ty_T + \Omega\frac{4\mu+m}{2m}x_0y_0 \\
&-\Omega((\frac{\mu^2}{m^2\nu}+\frac{\mu^2}{m^2})(x_T+x_0)(y_T+y_0)) \\
&-2\Omega\int_0^T dteE_x(t)(y_TG_1(t)+y_0G_2(t)) \\
&-2y_T\Omega\int_0^T dteE_x(t)(\frac{\mu\sin\nu(T-t)}{m^2\nu}+\frac{\mu(T-t)}{mM}) \\
&+x_T\int_0^T dtE_x(t)(\frac{\mu}{m}[\frac{\sin\nu t}{\sin\nu T}-\frac{\sin\frac{\nu}{2}(T-t)\sin\frac{\nu}{2}t}{\cos\frac{\nu}{2}T}]+\frac{\mu t}{MT}) \\
&+x_0\int_0^T dtE_x(t)(\frac{\mu}{m}[\frac{\sin\nu(T-t)}{\sin\nu T}-\frac{\sin\frac{\nu}{2}(T-t)\sin\frac{\nu}{2}t}{\cos\frac{\nu}{2}T}]+\frac{\mu(T-t)}{MT}) \\
&-e^2\int_0^T\int_0^T dtdsE_x(t)E_x(s)(\frac{\mu^2}{m^2}[\frac{\sin\nu(T-t)\sin\nu s}{\nu\sin\nu T} \\
&-\frac{4\sin\frac{\nu}{2}(T-t)\sin\frac{\nu}{2}t\sin\frac{\nu}{2}(T-s)\sin\frac{\nu}{2}s}{\nu\sin\nu T}]+\frac{\mu(T-t)s}{MT})\Big\}.
\end{aligned} \tag{4.47}$$

4.2 The Propagator in Limiting Cases

The main quantity of the calculation in this chapter is the two-dimensional propagator of an electron in the transverse magnetic field and the x-direction electric field with a two-parameter nonlocal harmonic potential energy. In this section, we consider the propagator in the limiting cases.

Absence of Magnetic Field

In this case, the transverse magnetic field approaches zero. We consider the system of interest corresponding to $\omega \to 0$ or equivalently $M \to \infty$. We first consider the prefactor in equation (4.47). In the case

$$\lim_{\omega\to 0} F(T) = \lim_{\omega\to 0} \frac{m}{2\pi i\hbar T}\left(\frac{\nu \sin\frac{\omega}{2}T}{\omega \sin\frac{\nu}{2}T}\right)^2.$$

According to equation (4.41), if the force constant (κ) approaches to zero then the relative harmonic frequency (ν) is equal to the harmonic frequency (ω). Thus, the prefactor is

$$F(T) = \frac{m}{2\pi i\hbar T}\left(\frac{\omega T}{2\sin\frac{\omega}{2}T}\right)^2. \tag{4.48}$$

We consider in the limit $M \to \infty$, the classical path becomes

$$\begin{aligned} S_{cl}^f = &\left(\frac{m\omega}{4}\cot\frac{\omega}{2}T\right)|(x_T - x_0)^2 + (y_T - y_0)^2| \\ &+x_T\int_0^T dteE_x(t)\left(\frac{\sin\omega t - 2\sin\frac{\omega}{2}T\sin\frac{\omega}{2}(T-t)\sin\frac{\omega}{2}t}{\sin\omega T}\right) \\ &+x_0\int_0^T dteE_x(t)\left(\frac{\sin\omega t - 2\sin\frac{\omega}{2}T\sin\frac{\omega}{2}(T-t)\sin\frac{\omega}{2}t}{\sin\omega T}\right) \\ &-e^2\int_0^T\int_0^T dtdsE_x(t)E_x(s)(\frac{\sin\omega(T-t)\sin\omega s}{\omega\sin\omega T}. \end{aligned}$$

$$-\frac{4\sin\frac{\omega}{2}(T-t)\sin\frac{\omega}{2}t\sin\frac{\omega}{2}(T-s)\sin\frac{\omega}{2}s}{\omega\sin\omega T}). \tag{4.49}$$

Recalling that the Feynman propagator expression,

$$K(x_T, y_T, T; x_0, y_0, 0) = F(T)\exp\left(\frac{i}{\hbar}S_{cl}\right),$$

it is the exact propagator of an electron moving in two dimensions under the x-direction electric field and a one-parameter nonlocal harmonic potential [8].

Absence of Electric Field

If the electric field $\vec{E}_x(t) \to 0$, then the propagator reduces to

$$K(x_T, y_T, T; x_0, y_0, 0) = \frac{m}{2\pi i\hbar T}\left(\frac{\omega T}{2\sin\frac{\omega}{2}T}\right)^2$$

$$\exp\frac{i}{\hbar}\left(\frac{m\omega}{4}\cot\frac{\omega}{2}T|(x_T-x_0)^2+(y_T-y_0)^2|\right). \tag{4.50}$$

This expression is the two-dimensional propagator of an electron in a one-parameter nonlocal harmonic potential energy.

Absence of Nonlocal Field

When the nonlocal harmonic potential goes to zero, the system of interest corresponds to the case when a relative harmonic frequency $\nu \to 0$. The propagator reduces to the simple form of

$$K(x_T, y_T, T; x_0, y_0, 0) = (\frac{m}{2\pi i\hbar T})\exp\frac{i}{\hbar}\left(\frac{m^*}{2T}|(x_T-x_0)^2+(y_T-y_0)^2|\right), \tag{4.51}$$

where $m^* = m\mu/M$ is defined as the effective mass. This is a free particle propagator.

4.3 Summary

The exact propagator for an electron moving in a two-dimensional system under the influence of a magnetic field and an electric field with a one-parameter nonlocal harmonic potential was calculated by Samathiyakanit [8] and Sa-yakanit et al. [40].

In this work, we generalize the model of random potential by introducing the nonlocal harmonic random potential with two parameters. The exact two-dimensional propagator in the transverse magnetic field and the x-direction electric field with a two-parameter nonlocal harmonic random potential cannot be evaluated exactly. Because the equation of motion is a set of coupled integro-differential equations due to the symmetric gauge, it cannot be solved exactly by the above methods.

However, we apply the first-order cumulant approximation to calculate the problem. The cumulant approximation is

$$\langle \exp[X] \rangle = \exp\left\{ \langle X \rangle + \frac{1}{2}(\langle X^2 \rangle - \langle X \rangle^2) + ... \right\}.$$

If we keep only the first-order term, then the first-order cumulant approximation becomes $\langle e^X \rangle \sim e^{\langle X \rangle}$. Therefore, the first-order cumulant approximation neglects the quantum fluctuation around the mean value. The propagator can be calculated by separating the Lagrangian into the x- and y-components. The x-component propagator can be calculated exactly using the two-particle system method but the y-component propagator cannot be evaluated exactly. We use the first-order cumulant approximation to approximate the classical action of the y-component and we calculate $\langle y(t) \rangle_{S_0}$ and $\langle y(t)y(s) \rangle_{S_0}$ by using the generating functional method [22]. Therefore, the propagator is a product of the

x-component and y-component propagators; nevertheless, the expression is more complicated.

Finally, we consider the two-dimensional propagator in the limiting cases. For the case of the absence of the magnetic field, the propagator of a two-parameter random potential reduces to a close form of the one-parameter random potential that can be calculated by Samathiyakanit [8]. The two-parameter result becomes more general than the one-parameter result; moreover, it can be reduced to the one-parameter result by taking the limit $M \to \infty$. In the cases of absence of the electric field and the nonlocal harmonic potential, the propagator can be reduced to the nonlocal harmonic propagator and the free particle propagator, respectively.

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Chapter 5
Density of States

In this chapter we will calculate the density of states in a random system. The variational path integral method can be used for calculating the approximated density of states. In the next section, a comparison between two-dimensional density of states (2D DOS) from the path integral and the result of white noise limit is discussed. The result using the two-parameter trial action will be compared with the one-parameter.

5.1 Introduction

The problem of an electron in a disordered system at a high density limit (HDL) has been interested by physicists for five decades. The important example is heavily doped semiconductors, as impurity ions have very high density. Kane [27] has applied the semiclassical or Thomas-Fermi type approximation to calculate DOS in the high energy limit. In the semiclassical approximation(SA), the potential fluctuation caused by charged impurities are assumed to be smooth [28]. The electron only feels the potential of the point where it locates. In the low energy limit, Halperin and Lax [29] introduced the potential fluctuation caused by the quantum effects. In the regions of deep narrow potential wells the electrons will be highly localized. This is the band tail of DOS. However, Sa-yakanit [5], and Sa-yakanit and Glyde [6] has introduced the Feynman path-integral method to calculated the DOS in the cases, i.e., the Gaussian random potential and the screened Coulomb potential. His resulting density of states is valid at all energy

limits. In the low energy limit it can be expressed in an analytic form which is the same as proposed by Halperin and Lax [29] and in the high energies limit it is analogous to the semiclassical Kane's result [27].

In this work we consider an electron confined in two-dimensional disorder systems. The impurity in the system produces the random potential interacting with an electron. The aim of the present work is to analyze the fluctuation potentials which can be expressed in the Gaussian correlation function. The two-dimensional density of states (2D DOS) has been treated within the variational Feynman path integral with a two-parameter nonlocal harmonic trial action. In high energy limit, the 2D DOS has been expressed in an analytic form by letting $t \to 0$, which is the assumption of the semiclassical approximation. In the asymptotic approximation, the analytic 2D DOS reduces to a free electron DOS and the Gaussian band tail, which agrees with Kane's result. In the case of the low energy limit, the 2D DOS is expressed in the analytic form with the dimensionless functions of the preexponential factor $a(\upsilon, \rho)$ and the exponential $b(\upsilon, \rho)$, respectively that the expression of 2D DOS is analogous with the result of Halperin and Lax in low energies.

5.2 Density of States for a Random System

The density of states $N(E)$ is the total number of energy eigenstates in the interval $[E, E + dE]$ and can be represented as

$$n(E) = \frac{1}{V} \sum_{n=1}^{\infty} \delta(E - E_n), \tag{5.1}$$

when E_n is the energy of the nth eigenstate, V is the volume of the system. If the system is disordered, we must average equation (2.41) over the statistical ensemble

for the random potential. It is convenient to consider the density of states in the form of equation (2.41). In order to apply the path integral formulation to equation (2.41), one converts equation (5.1) into

$$n(E) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} TrK(x^{''}, T; x^{'}, 0)\exp[\frac{i}{\hbar}Et]dt \tag{5.2}$$

where the operator Tr denotes the trace of propagator K. The propagator is a retarded propagator describing the propagation of an electron from point $x^{''}$ to point $x^{'}$. If the propagator K is invariant under translation of x, then

$$K(x^{''}, T; x^{'}, 0) = K(x^{''} - x^{'}; T, 0). \tag{5.3}$$

To find the density of states, the end point and initial point must be the same. Therefore,

$$n(E) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} K(0, 0; T, 0)\exp[\frac{i}{\hbar}Et]dt. \tag{5.4}$$

5.2.1 The Approximate Propagator

The two-dimensional random system in the Edward-Gulayev's model is considered in the limit of a set of N rigid scatterers confined randomly within a volume V in a surface space. The density, n, of the scatterer is high but the potential between an electron and a scatterer, $v(\vec{r}(t) - \vec{R})$, is weak. The system can be viewed as an electron moving in the average scattering potential by expressing the autocorrelation function, the action of this system is

$$S[\vec{r}(t)] = \int_0^T dt\left[\frac{m}{2}\dot{\vec{r}}^2(t) - E_0 + \frac{in\eta^2}{2\hbar}\int_0^T dsW(\vec{r}(t) - \vec{r}(s))\right], \tag{5.5}$$

where $\vec{r}(t)$ are two dimension coordinates. The E_0 is the average potential energy, which is defined as $E_0 = \langle v(\vec{r}) \rangle$, and the parameter η represents the weakness of the scattering potential and it is explicitly written to indicate the dimensions involved. For the case of interest, the scatterers random distribution can be described by the Gaussian distribution. An electron moving in weak and dense receptors is equivalent to moving in the Gaussian potential. The autocorrelation [30] has the form

$$W(\vec{r}(t) - \vec{r}(s)) = u^2(\pi L^2)^{-1} \exp\left(-\frac{|\vec{r}(t) - \vec{r}(s)|^2}{L^2}\right) \tag{5.6}$$

where L is the Gaussian correlation length of the random system and u is another parameter which takes care the dimensionality of the system.

In general, a lot of path integrals cannot be integrated out and our problem is one of these cases. The most widely used methods in path integral formalism is a variational method. The concept of this method is that the appropriate trial action with parameter can be obtained with high accuracy. There are two basic idea that indicate whether the chosen trial action is suitable or not. First, this action should be carried out easily and exactly. Second, the physical meaning of the of the real system and the trial action must be likely. Therefore, we use the variational method which we can adjust appropriate trial action. In this investigation, we follow the method given by Samathiyakanit [8]. He introduced a two-parameter nonlocal harmonic trial action with ω and κ, which is

$$S_0(\kappa, \omega) = \int_0^T dt \frac{m}{2} \dot{\vec{r}}^2(t) - \frac{\kappa\omega}{8} \int_0^T \int_0^T dt ds (\vec{r}(t) - \vec{r}(s))^2 \frac{\cos\omega(\frac{T}{2} - |t - s|)}{\sin\frac{\omega}{2}T}, \tag{5.7}$$

where κ, ω are the the forced constant and harmonic frequency respectively. This trial action is the action of a two-particles model system. The idea of this model is

that a set of scatterers is dense and can be approximated by one-particle oscillator with frequency, ω, at the same time its coupling with a free electron by forced constant, κ. The average propagator is written as

$$K_1(\vec{r}_T, \vec{r}_0; T) = K_0(\vec{r}_0, \vec{r}_0; T) \left\langle \exp\left[\frac{i}{\hbar}(S - S_0(\kappa, \omega))\right] \right\rangle_{S_0(\kappa,\omega)} \tag{5.8}$$

where a non-local harmonic oscillator has

$$K_0(\vec{r}_0, \vec{r}_0; T) = \int D[\vec{r}(t)] \exp \frac{i}{\hbar} S_0[\vec{r}(t)],$$

and the average $\langle . \rangle_{S_0(\kappa,\omega)}$ is defined in equation (4.21). Consequently, we approximate the equation (5.8) by using the first-order cumulant expansion [24]. The average propagator can be rewritten as

$$K_1(\vec{r}_T, \vec{r}_0; T) = K_0(\vec{r}_0, \vec{r}_0; T) \exp\left[\frac{i}{\hbar}(\langle S \rangle_{S_0(\kappa,\omega)} - \langle S_0 \rangle_{S_0(\kappa,\omega)})\right], \tag{5.9}$$

where the index 1 denotes the first-order cumulant approximation. To evaluate $K_1(\vec{r}_T, \vec{r}_0; T)$, we have to find $K_0(\vec{r}_0, \vec{r}_0; T)$, $\langle S \rangle_{S_0(\kappa,\omega)}$ and $\langle S_0 \rangle_{S_0(\kappa,\omega)}$ since the kinetic term is always cancelled out from the average. The $K_0(\vec{r}_0, \vec{r}_0; T)$ can be carried out in previous chapter by taking translation invariant

$$\begin{aligned} K_0(\vec{r}_0, \vec{r}_0; T) &= F(\nu, \omega, T) \exp[\frac{i}{\hbar} S_{0,Cl}(\vec{r}_T - \vec{r}_0, T)] \\ &= \frac{1}{2\pi i\hbar T} \left(\frac{\nu \sin \frac{1}{2}\omega T}{\omega \sin \frac{1}{2}\nu T} \right)^2. \end{aligned} \tag{5.10}$$

The average $\langle S \rangle_{S_0(\kappa,\omega)}$ can be evaluated by making a Fourier transform of autocorrelation function $W(\vec{r}(t) - \vec{r}(s))$ and the expression (5.10) can be used to evaluate $\langle S_0 \rangle_{S_0(\kappa,\omega)}$. Thus we can write

$$\langle S \rangle_{S_0(\kappa,\omega)} = -E_0 T + \frac{in\eta^2}{2\hbar} \int_0^T \int_0^T dt ds \langle W(\vec{r}(t) - \vec{r}(s)) \rangle_{S_0(\kappa,\omega)} \tag{5.11}$$

where $W(\vec{r}(t)-\vec{r}(s))$ is given by equation (5.6) for the Gaussian potential. This average is difficult to carry out the average of the Gaussian potential. We have better use its Fourier transform in the two dimensional system,

$$W(\vec{r}(t)-\vec{r}(s)) = \int \frac{d\vec{k}}{(2\pi)^2} W(\vec{k}) \exp[i\vec{k}\cdot(\vec{r}(t)-\vec{r}(s))] \tag{5.12}$$

where

$$W(\vec{k}) = u^2 \exp\left[-\frac{L^2}{4}\vec{k}^2\right]. \tag{5.13}$$

We can rewrite the average $\langle S\rangle_{S_0(\kappa,\omega)}$ by taking the Fourier transform of the autocorrelation function as

$$\langle S\rangle_{S_0(\kappa,\omega)} = \frac{in\eta^2u^2}{2\hbar}\int_0^T\int_0^T dtds \int \frac{d\vec{k}}{(2\pi)^2}\exp\left\{-A\vec{k}^2 + i\vec{B}\cdot\vec{k}\right\} \tag{5.14}$$

where the defined parameters are

$$A = \{\frac{L^2}{4} + \frac{1}{2}[\frac{1}{2}\langle(\vec{r}(t)-\vec{r}(s))^2\rangle_{S_0(\kappa,\omega)} - \langle r(t)-r(s)\rangle^2_{S_0(\kappa,\omega)}]\}$$

$$\vec{B} = \langle\vec{r}(t)-\vec{r}(s)\rangle_{S_0(\kappa,\omega)}. \tag{5.15}$$

For the Gaussian case, we apply the Gaussian integration formula for equation (5.14) and for each cartesian coordinate of $\vec{k}$-integration. The we obtain

$$\langle S\rangle_{S_0(\kappa,\omega)} = -E_0T + \frac{in\eta^2}{8\pi\hbar}\int_0^T\int_0^T dtdsA^{-1}\exp\left(-\frac{\vec{B}^2}{4A}\right), \tag{5.16}$$

where the parameters in an above equation can be solved explicitly in [8], by using

$$A = \{\frac{L^2}{4} + i\hbar\frac{\mu}{m^2\nu}(\frac{\sin\nu(T-|t-s|)/2\sin\nu(t-s)/2}{\sin\nu T/2} + \frac{(T-(t-s))(t-s)}{2MT})\}$$

$$\vec{B} = \{\frac{\mu \sin \nu(t-s)/2 \cos \nu(T-|t-s|)/2}{m \sin \nu T/2} + \frac{\mu(t-s)}{MT}\}(\vec{r}_T - \vec{r}_0). \tag{5.17}$$

Next, we evaluate $\langle S_0 \rangle_{S_0(\kappa,\omega)}$ by employing the identity in equation (4.51) and setting ω equal to a constant

$$\frac{i}{\hbar}\langle S_0 \rangle_{S_0(\kappa,\omega)} = \kappa \frac{\delta \ln K_0}{\delta \kappa}|_{\omega=constant}, \tag{5.18}$$

where

$$K_0 = F(T) \exp\ \left[\frac{\mu\nu}{4} \cot \frac{\nu}{2}T + \frac{m\mu}{2MT}\right](\vec{r}_T - \vec{r}_0)^2, \tag{5.19}$$

and

$$F(T) = \frac{m}{2\pi i\hbar T}\left(\frac{\nu \sin \frac{\omega}{2}T}{\omega \sin \frac{\nu}{2}T}\right)^2. \tag{5.20}$$

Using equations (5.19),(5.20) and carrying out the differentiation in equation (5.18), we obtain

$$\frac{i}{\hbar}\langle S_0 \rangle_{S_0(\kappa,\omega)} = \frac{i}{\hbar}\frac{\mu^2}{2m}\left\{\frac{\nu T}{2}(1+\frac{2m}{M}) \cot \frac{\nu}{2}T - (\frac{1}{2}\nu T \csc \frac{\nu}{2}T)^2 - \frac{2m}{M}\right\} \cdot \frac{(\vec{r}_T - \vec{r}_0)^2}{2T}$$

$$-\frac{\mu}{m}\left(\frac{\nu T}{2} \cot \frac{\nu}{2}T - 1\right). \tag{5.21}$$

5.2.2 The Approximation of the Density of States

The approximated density of states for a random system can be calculated by following the same procedure in equation (5.5) and substituting equations (5.16), (5.17) and (5.21) into the average propagator $K_1(r_T, r_0; T)$ in equation (5.9). Next, we take the trace of the average propagator which is we set $\vec{r}_T = \vec{r}_0$ and substitute in the expression of the density of states, we get

$$N_1(E) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dT \left(\frac{m}{2\pi i\hbar T}\right)\left(\frac{\nu \sin \frac{\omega}{2}T}{\omega \sin \frac{\nu}{2}T}\right)^2$$

$$\exp\left\{\frac{i}{\hbar}(E-E_0)T+\frac{\mu}{m}\left(\frac{\nu T}{2}\cot\frac{\nu}{2}T-1\right)\right.$$
$$-\frac{\xi_L^{'}}{2\hbar^2}\int_0^T\int_0^T dtds\{\frac{L^2}{4}+i\hbar\frac{\mu}{m}(\frac{\sin\nu(t-s)/2\sin\nu(T-|t-s|)/2}{m\nu\sin\nu T/2}$$
$$\left.+\frac{(T-|t-s|)(t-s)}{2MT})\}^{-1}\right\}, \tag{5.22}$$

where $\xi_L^{'}=nu^2\eta^2$. Note that the periodic function, J, has the property

$$J(|t-s|)=J(T-|t-s|),$$

the double-time integration can be reduced to a single integration [31], change integral by set $x=t-s$ and obtain

$$\int_0^T\int_0^T dtds[J(T-|t-s|)+c]^{-1}=T\int_0^T dx[J(x)+c]^{-1}. \tag{5.23}$$

If, we define the variable

$$\rho=\sqrt{m/(m+M)}, \tag{5.24}$$

then we have the relation $\omega=\nu\rho$ and $\mu/m=1-\rho^2$. The variational parameters (ω,κ) can be converted by the new variational parameters that are the relative harmonic frequency ν and a parameter ρ, respectively. The density of states can be rewritten as

$$N_1(E)=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}dT\left(\frac{m}{2\pi i\hbar T}\right)\left(\frac{\sin\frac{1}{2}\rho\nu T}{\rho\sin\frac{\nu}{2}T}\right)^2\exp\left\{\frac{i}{\hbar}(E-E_0)T\right.$$
$$\left.+(1-\rho^2)\left(\frac{\nu T}{2}\cot\frac{\nu}{2}T-1\right)-\frac{\xi_L^{'}}{2\hbar^2}T\int_0^T dxJ(x,\rho)^{-1}\right\}, \tag{5.25}$$

where

$$J(x,\rho)=\left\{\frac{L^2}{4}+i\hbar(1-\rho^2)(\frac{\sin\nu x/2\sin\nu(T-x)/2}{m\nu\sin\nu T/2})+\frac{i\hbar\rho^2}{2m}\frac{(T-x)x}{T}\right\}. \quad (5.26)$$

However, the obtained density of states is still too complicated and cannot be calculated exactly. Therefore, we consider it in the asymptotic approximation for the low energy and high energy limits. At large negative energies deep in the band tail ($E\to-\infty$), it is the so-called "quantum case" or "full-ground-state". The other limiting case ($E\to\infty$) corresponds to a "classical well". Therefore, two analytic expressions for the two-dimensional density of states can be obtained from the above expression and they are called the low energy limit and high energy limits.

Low Energy Limit

In the low energy band tail, the density of states is the contribution of the ground state energy. Thus we let $T\to\infty$ [6] and suppose that ρ is large. Hence, we are able to approximate [32],

$$\frac{\sin\nu x/2\sin\nu(T-x)/2}{\sin\nu T/2}\approx\frac{1}{2i},$$

$$\sin\rho\nu T/2\approx\frac{1}{2}\rho\nu T,$$

$$\sin\nu T/2\approx\frac{1}{2i}e^{i\nu T/2},$$

$$\left(\frac{\nu T}{2}\cot\nu T/2-1\right)\approx\frac{i\nu T}{2}. \quad (5.27)$$

Since, we substitute equation (5.27) into equation (5.25) and integrate by keeping only the term up to T^2, then the density of states becomes

$$N_{1L}(E) = \frac{1}{2\pi\hbar}\left(\frac{m}{2\pi\hbar}\right)\nu^2 \int_{-\infty}^{\infty} dT(iT)\exp\left\{\frac{i}{\hbar}\left((E-E_0) - E_\nu + \frac{1}{2}E_\nu(1-\rho^2)\right)T \right.$$
$$\left. -\frac{T^2}{2\hbar^2}\xi_L\left(1+4\frac{E_L}{E_\nu}(1-\rho^2)\right)^{-1}\right\}, \tag{5.28}$$

where $E_\nu = \hbar\nu$, $E_L = \hbar^2/2mL^2$ is the energy associated with localizing an electron within the correlation length and the fluctuation energy $\xi_L = 4\xi_L^{'}/L^2$ is the dimension of the energy squared. Using the formula [33] and the parabolic cylinder function, $D_p(z)$, we get

$$\int_{-\infty}^{\infty} dt(it)^p \exp(-\beta^2 t^2 - iqt) = \frac{\sqrt{\pi}}{2^{p/2}\beta^{p+1}}\exp(\frac{-q^2}{8\beta^2})D_p(\frac{q}{\beta\sqrt{2}}). \tag{5.29}$$

Therefore, the density of states can be written in an analytic form as

$$N_{1L}(E) = \frac{m}{(2\pi\hbar)^2}\frac{\sqrt{\pi}E_\nu^2}{\sqrt{2}\hbar}\left[\frac{\xi_L}{2\hbar^2}(1+4\frac{E_L}{E_\nu}(1-\rho^2))^{-1}\right]^{-1}$$
$$\times\exp\left(-\frac{(E-E_0-E_\nu+\frac{1}{2}E_\nu(1-\rho^2))^2}{4\xi_L(1+4\frac{E_L}{E_\nu}(1-\rho^2))^{-1}}\right)$$
$$\times D_1\left(-\frac{E-E_0-E_\nu+\frac{1}{2}E_\nu(1-\rho^2)}{\sqrt{\xi_L}(1+4\frac{E_L}{E_\nu}(1-\rho^2))^{-1/2}}\right). \tag{5.30}$$

Let define the energy dimensionless parameters $\upsilon = (E_0 - E)/E_L$, $x = E_\nu/E_L$ and $x^{'} = E_\nu(1-\rho^2)/E_L$. Now we are interested in the density of states in the deep band tail. This can be achieved by letting $E \to -\infty (q \to \infty)$ and using the asymptotic expansion of the parabolic cylinder function [33],

$$D_p(x) = \mathrm{e}^{-x^2/4}x^p\left(1 - \frac{p(p-1)}{2x^2} + ...\right). \tag{5.31}$$

For large argument values, $D_1(x) \sim x\mathrm{e}^{-x^2/4}$, we obtain the asymptotic expression with dimensionless parameter for the low energy density of states as

$$N_{1L}(E) = \frac{(E_L/L^2)^2}{\xi_L^{3/2}} a(\upsilon, x, x^{'}) \exp\left(\frac{-b(\upsilon, x, x^{'})E_L^2}{2\xi_L}\right), \tag{5.32}$$

where the dimensionless parameters are

$$a(\upsilon, x, x^{'}) = \frac{1}{2^{5/2}\pi^{3/2}} x^2(\upsilon + x - \frac{1}{2}x^{'})(1 + \frac{4}{x^{'}})^{3/2} \tag{5.33}$$

$$b(\upsilon, x, x^{'}) = (\upsilon + x - \frac{1}{2}x^{'})^2(1 + \frac{4}{x^{'}}). \tag{5.34}$$

The 2D DOS in the low energy limit is analogous with that proposed by Halperin and Lax [29]. This DOS is proportional to the dimensionless parameters $a(\upsilon, x, x^{'})$ and $b(\upsilon, x, x^{'})$, respectively.

High Energy Limit

In high energy limit case, it is necessary to take the limit $T \to 0$ [6] or equivalently $\rho \to 0$, which we can neglect the ρ^2 term. Thus we are able to approximate

$$\frac{\sin \nu x/2 \sin \nu(T-x)/2}{\sin \nu T/2} \approx 0,$$

$$\left(\frac{\sin \rho\nu T/2}{\rho \sin \nu T/2}\right)^2 \approx 1,$$

$$\left(\frac{\nu T}{2}\cot \nu T/2 - 1\right) \approx 0. \tag{5.35}$$

Inserting equation (5.35) into equation (5.25), we obtain

$$N_{1H}(E) = \frac{1}{2\pi\hbar}\left(\frac{m}{2\pi\hbar}\right)\int_{-\infty}^{\infty} dT(iT)^{-1} \exp\left\{-\frac{i}{\hbar}(E_0 - E)T - \frac{T^2}{2\hbar^2}\xi_L\right\}. \tag{5.36}$$

By using the parabolic cylinder function and the condition of the low energy limit, the density of states in high energy limit becomes

$$N_{1H}(E) = \frac{2m}{(2\pi)^{3/2}\hbar^2} \mathrm{e}^{-(E_0-E)^2/4\xi_L} D_{-1}\left(\frac{(E_0-E)}{\sqrt{\xi_L}}\right). \tag{5.37}$$

This is analogous with the semiclassical Kane's result [27] for the two dimensional density of states. Using the asymptotic expansion of parabolic cylinder function for a large negative argument [34], $D_{-1}(x) \sim \sqrt{\pi/2} \cdot e^{x^2/4}[1 + \mathrm{erf}(x)]$, we get the following expression for the two dimensional free electron density of states in terms of the error function

$$N_{1H}(E) = \frac{m}{2\pi\hbar^2}\left(1 + \mathrm{erf}\left(\frac{E-E_0}{\sqrt{\xi_L}}\right)\right). \tag{5.38}$$

This equation for the density of states is analogous to Van Mieghem's result [34].

Let us consider two limiting cases for positive and negative $E_0 - E$. From the analytic expression in equation (5.37) using the asymptotic representation of the parabolic cylinder function for $E \ll E_0$ [35], $D_{-1}(x) \sim e^{-x^2/4}/x$ for $|x| \ll -1$ and we take the error function in equation (5.38) for $E \gg E_0$ [35], we obtain the asymptotic density of states

$$N_{1H}(E) = \begin{cases} \dfrac{m}{\pi^{3/2}\hbar^2}\dfrac{\sqrt{\xi}}{\sqrt{2}(E_0-E)}\mathrm{e}^{-(E_0-E)^2/2\xi_L} & : \quad (E-E_0) \ll -1 \\ \dfrac{m}{\pi\hbar^2} & : \quad (E-E_0) \gg 1 \end{cases}. \tag{5.39}$$

The first of these expressions is the band tail result of Kane for a two dimensional problem and the second is well known free electron band valid for a positive $(E - E_0)$.

We also plot the normalized analytic DOS and the free electron DOS on the same plot as shown in Figure 5.1. The tail shows localized states of electrons.

Heavily doped semiconductors have impurity localized energy levels in the band gap. At high densities, these localized energy levels interact and form a band, this impurity band merges with the conduction and the valence band. The impurity band is a band tail of the system. The asymptotic density of states for the two limits, the plots are shown in Figure 5.2. These curves represent the normalized analytic DOS and the normalized asymptotic DOS.

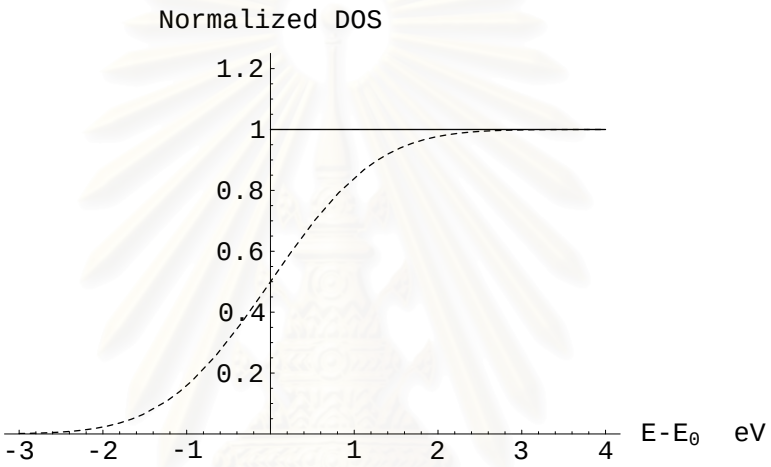

Figure 5.1: The normalized analytic DOS in equation (5.37) (dash line) with a normalized free electron gas DOS (solid line).

5.3 Comparison of Results

In this section, the results of 2D DOS in the previous section are compared with the results calculated by Sa-yakanit and Slavcheva [36], and Sa-yakanit et al. [37] and the result of tight-binding simulation in the white noise limit [38]. The white noise limit, the correlation length (L) of the Gaussian random potential approaches zero, that is a delta function potential.

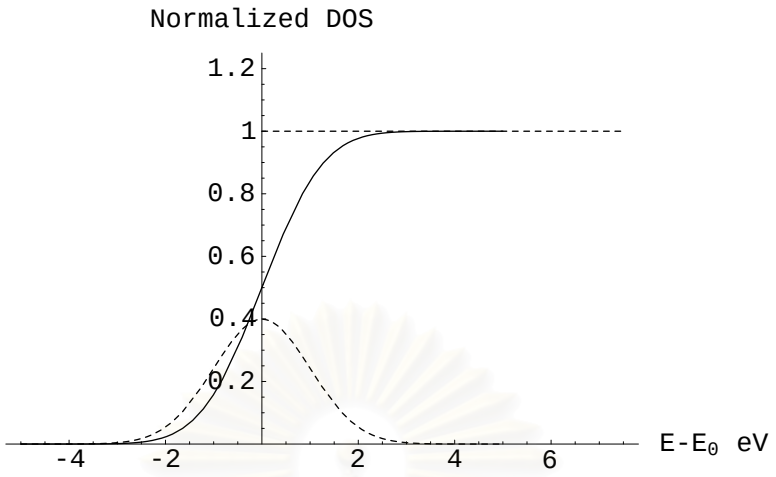

Figure 5.2: Plot of the normalized analytic DOS (solid line) and the normalized asymptotic DOS (dash line).

5.3.1 Comparison 2D DOS Between 1P with 2P Variational Path Integrals

The DOS in equation (5.32) has been calculated by the variational path integral with the the two variational parameters (2P) that are ν, ρ, respectively.

In order to account for the variational parameters that introduced to minimize the argument of the exponential in DOS or equivalently to maximize DOS [39]. First, we choose ν which maximizes DOS, by differentiating dimensionless $b(\upsilon, x, x^{'})$ with respect to x and letting it equal to zero [29]. The variable x is the ratio of the energy associating with the harmonic oscillator and the correlation energy. The Gaussian case, the best choice of x is kept only the positive roots that is satisfy the equation

$$x^2 - \frac{4\upsilon}{(1+\rho^2)^2} + \frac{4\upsilon\rho^4}{(1+\rho^2)^2} + \frac{2x(1-\rho^4)}{1+\rho^2} = 0. \tag{5.40}$$

In the white noise limit, $L \to 0$. This implies that $x = 2mL^2\nu/\hbar$ is vanishingly

small. Neglecting x^2 corresponds to neglecting the fluctuation in $W(\vec{r})$ within its correlation length L, then we can write

$$x = \frac{2\upsilon}{1+\rho^2}, \tag{5.41}$$

and we introduce the dimensionless fluctuation energy as

$$\xi' = \frac{\xi_L}{E_L^2}. \tag{5.42}$$

We substitute equations (5.41), (5.42) into equation (5.32) and normalize it with respect to the 2D free electron DOS. At the same time we apply the dimensionless expression in equations (5.33) and (5.34), then the normalized 2D-DOS can be written as

$$\frac{N_{1L}^{2P}(\upsilon)}{N_0} = \left(\frac{2\pi}{\xi'^{3/2}}\right) a(\upsilon,\rho) e^{-b(\upsilon,\rho)/2\xi'}, \tag{5.43}$$

where

$$a(\upsilon,\rho) = \frac{1}{2^{5/2}\pi^{3/2}} \frac{(2\upsilon)^3}{(1+\rho^2)^2} \left(1 + \frac{4(1+\rho^2)}{2\upsilon(1-\rho^2)}\right)^{3/2}, \tag{5.44}$$

$$b(\upsilon,\rho) = (2\upsilon)^2 \left(1 + \frac{4(1+\rho^2)}{2\upsilon(1-\rho^2)}\right). \tag{5.45}$$

For the 2D-DOS with dimensionless parameter in the band tail has been calculated by Sa-yakanit and Slavcheva [36], using the variational path integral method with the one-parameter trial action. The normalized 2D-DOS in the white noise limit is

$$\frac{N_{1L}^{1P}(\upsilon)}{N_0} = \left(\frac{2\pi}{\xi'^{3/2}}\right) a(\upsilon) e^{-b(\upsilon)/2\xi'}, \tag{5.46}$$

where

$$a(\upsilon) = \frac{1}{2^{5/2}\pi^{3/2}}(2\upsilon)^3(1+\frac{4}{2\upsilon})^{3/2}, \tag{5.47}$$

$$b(\upsilon) = (2\upsilon)^2(1+\frac{4}{2\upsilon}). \tag{5.48}$$

In fact, the parameter ρ is proportional to the mass M. According to equation (5.24), if $M \to \infty$ then the parameter $\rho^2 \to 0$. Therefore, the normalized 2D DOS in equation (5.43) reduces to the normalized 2D DOS of the one-parameter variational in equation (5.46) in the limit of $\rho^2 = 0$.

5.3.2 Comparison Path Integral Results in the White Noise Limit

The density of states of an electron in the white noise potential in two dimensions has been calculated by Thouless and Elzain [38]. The 2D-DOS in the white noise limit has been calculated by the coherent potential approximation (CPA) at high energies, it has also been calculated from the fluctuation theory in low-energy band tails. The result of a tight-binding (T-B) two-dimensional simulation with respect to the white noise problem in low energies is compared with the CPA in Figure 5.3. In addition, the tight-binding normalized 2D DOS for negative $E-E_0$ is the straight line, which fits well with the simple exponential

$$\frac{n^{T-B}(E)}{N_0} \approx 0.17 \exp\left[\frac{4\pi(0.931)(E-E_0)}{Q}\right] \tag{5.49}$$

where Q is energy scale of the white noise.

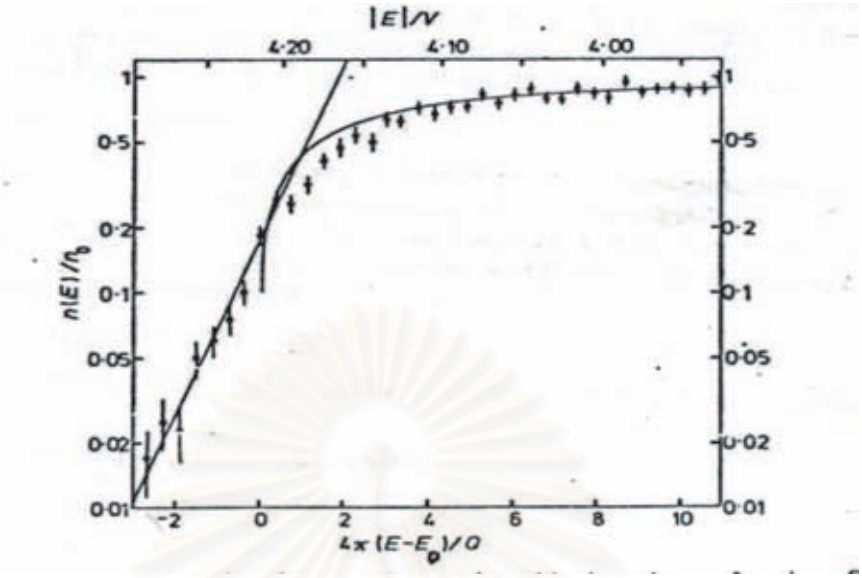

Figure 5.3 Normalized density of states $n(E)$on logarithm as a function of energy E. Their calculation results are shown with error bars. The curve gives the CPA density of states and the straight line the exponential tail of the tight-binding simulation.

This DOS is, however, independent of the dimensionless energy υ. We define Q proportional to the variance, $W^2 = \xi^{'}$, and the potential energy, $V = E_L$. Therefore, we can define a new dimensionless energy η as

$$\eta = \frac{4\pi(E - E_0)}{Q} = \frac{4\pi(E - E_0)}{E_L \xi'}. \tag{5.50}$$

Thus, the dimensionless energy can be rewritten in terms of the new parameter η as

$$\upsilon = \frac{\eta \xi^{'}}{4\pi}. \tag{5.51}$$

Therefore, the normalized 2D DOS in a Gaussian white noise limit can be written in terms of a new dimensionless energy as

$$\frac{n^{T-B}(\eta)}{N_0} \approx (0.17)\exp(0.931\eta)\,. \tag{5.52}$$

Referring to equations (5.43) and (4.46) in the white noise limit, they imply that x is very small and the dimensionless energy $\upsilon \ll 1$. We can express the normalized 2D DOS in terms of a new parameter η as

$$\frac{N_{1L}^{1P}(\eta)}{N_0} = \frac{2^3\eta}{\pi^{3/2}\xi'^{1/2}}\exp\left(-\frac{\eta}{4\pi}\right), \tag{5.53}$$

and

$$\frac{N_{1L}^{2P}(\eta)}{N_0} = \frac{2^3\eta}{\pi^{3/2}\xi'^{1/2}(1+\rho^2)^2}\exp\left(-\frac{\eta(1+\rho^2)}{4\pi(1-\rho^2)}\right), \tag{5.54}$$

where superscripts 1P and 2P are the case of the one- and two parameter trial actions, respectively.

We plot the two cases of the variational path integral results for the normalized 2D DOS on the same plot with the result of the tight-binding simulation [38] in the white noise limit as shown in Figure 5.4. From the work of Sa-yakanit and Glyde [6], the magnitude of the energy fluctuation ξ' is about 5 in n-GaAs. As it can be seen in the Figure 5.4 that the results from the two variational parameters of the path integral in the white noise limit with setting the variational parameter $\rho^2 = 0.15$ is closed to the tight-binding simulation point than that from the one-parameter variational path integral.

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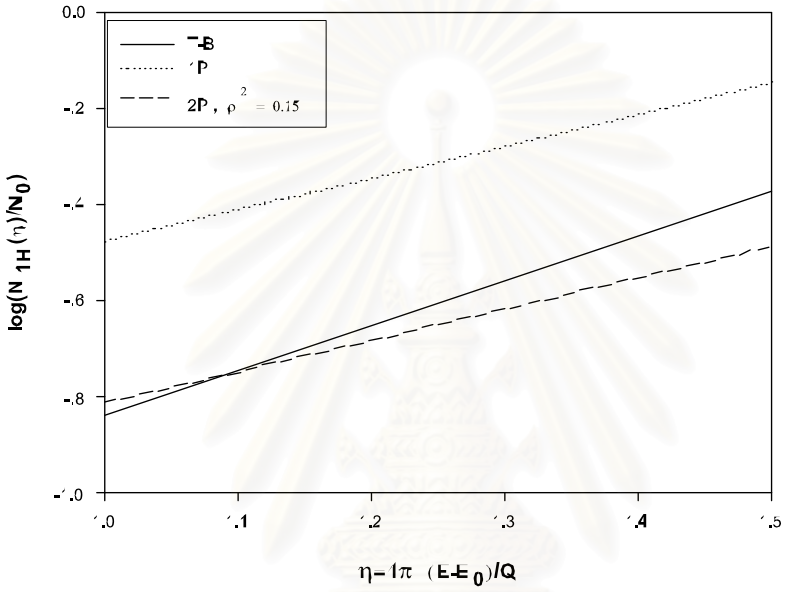

Figure 5.4 The normalizes 2D DOS on logarithm with a dimensionless energy η in the white noise limit for the fluctuation energy dimensionless of n-GaAs ($\xi^{'} = 5$) [6] : (T-B : the tight-binding energy simulation result), (1P : the one-parameter variation result), (2P, $\rho^2 = 0.15$: The two-parameter variation result).

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Chapter 6
Discussions and Conclusions

We shall begin with the summary of the main results obtained in this work. Discussions and comparison will then be considered intensively. The main point: we generalize the model of random potential by introducing the the two-parameter nonlocal harmonic random potential instead of the one-parameter nonlocal harmonic random potential.

The exact propagator for an electron moving in a two-dimensional system under the influence of a magnetic field and an electric field with a one-parameter nonlocal harmonic potential was calculated by Sa-yakanit et al. [40]. The actual problem is transformed into an electron moving in a magnetic field under the external electric field and the nonlocal harmonic force by using Stratonovich's transformation [42]. Nevertheless, the transformed problem is a set of coupled differential equations due to the symmetric gauge. Using the 2×2 matrices introducing by Papadopoulos and Jones [41], the set of coupled differential equation reduces to the matrix equation, without a coupled equation. After completing the routine evaluation, we obtain the exact propagator.

Firstly, we calculate the exact two-dimensional propagator of an electron in the transverse magnetic field and the x-direction electric field with a two-parameter nonlocal harmonic random potential. The problem cannot be solved exactly by the Stratonovich's transformation and the 2x2 matrices methods because the equation of motion is a set of coupled integro-difference equations. However, we apply the two-particle system method [8] and the first-order cumulant approximation [24] to carry out. The first-order cumulant approximation

is

$$\langle \mathrm{e}^{X} \rangle \sim \mathrm{e}^{\langle X \rangle}.$$

The high-order terms are neglected. This mean that the quantum fluctuations around the mean value have been neglected. Thus we separate the Lagrangian into the x- and y-components. The x-component propagator can be calculated exactly using the method of a two-body problem but the y-component propagator cannot be evaluated exactly. We use the first-order cumulant approximation to approximate the classical action of the y-component and we calculate $\langle y(t) \rangle_{S_0}$ and $\langle y(t)y(s) \rangle_{S_0}$ by using the generating functional method [25]. Therefore, the propagator is a product of the x-component and y-component propagators; nevertheless, the expression is more complicated. In the case of absence the transverse magnetic field, the propagator of a two-parameter random potential reduces to a close form of the one-parameter random potential [8] in the limit $M \to \infty$.

Secondly, the density of states for a system with the Gaussian random potential is calculated by using the two-parameter variational method via path integrals or so-called the two-parameter theory. The approximation is based on the first-order cumulant approximation. The density of states can be considered in the two energy limits, which are the high-energy and the low-energy limits. At the high-energy limit, the two-dimensional density of states (2D DOS) is obtained by letting the time variable $T \to 0$. The density of states is independent on the number of variational parameters. Therefore, the 2D DOS agrees exactly with those of the one variational parameter for Sa-yakanit and Slavcheva [36]; furthermore, it is similar to the semiclassical Kane result also. However, the density of states is proportional to the magnitude of fluctuation potential energy

(ξ_L). The influence of a fluctuation potential energy is to localized electrons at an electron energy $E < E_0$ as shown in Figure 6.1. The probability of finding localized electron states increases as the fluctuation potential energy increases.

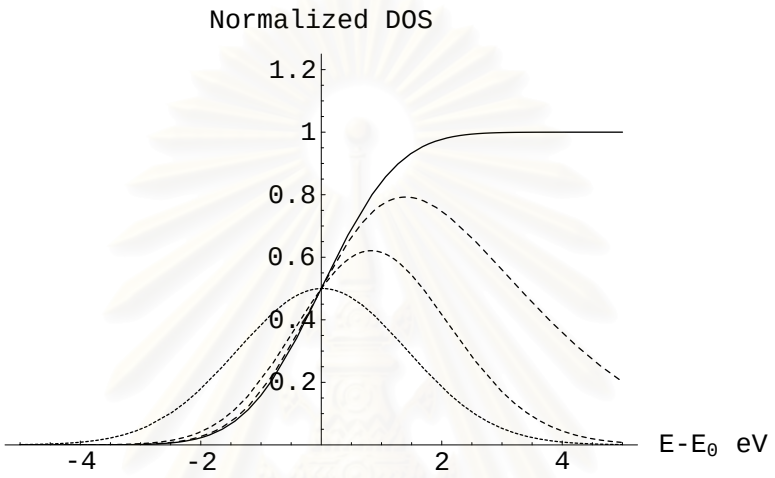

Fig.6.1 Plot of the normalized analytic DOS in a difference limits of the fluctuation potential energy $\xi_L(eV)^2$: (Solid line : $\xi_L = 1$), (Long dash line : $\xi_L = 1.1$), (Medium dash line : $\xi_L = 1.5$), (Short dash line : $\xi_L = 100$).

The low-energy limit can be reduced to the analytic density of states by taking $T \to \infty$. This means that only in the ground states will be retained in DOS. The asymptotic DOS ($E \to -\infty$) is proportional to the dimensionless parameters $a(\upsilon, x, x^{'})$ and $b(\upsilon, x, x^{'})$ given by equations (5.33) and (5.34), and clearly dependent on the parameters υ, x and ρ, where $x^{'}$ has been defined by $x^{'} = E_\nu(1-\rho^2)/E_L$. At the low energy limit or the full-ground state, 2D DOS from the two-parameter theory reduces to the one-parameter theory by letting $\rho^2 = 0$ or equivalent setting $x = x^{'}$.

Moreover, at the white noise limit the density of states in equation (5.54) is dependent on the parameter (ρ). The normalized DOS of two-parameter theory

is closer to the tight-banding simulation point than that from the one-parameter theory as shown in Figure 5.4. We see that the two-parameter theory is more advantageous than the one-parameter theory. Because, we can vary the variational parameters (x, ρ) to close the simulation result than the a one-parameter case. However, the two-parameter result can be reduced to the one-parameter result by letting $\rho^2 = 0$.

Finally, the result from the two-parameter theory becomes more general and covers the one-parameter condition. We may conclude that the two-parameter theory has improvement and advantages over the one-parameter theory.

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Appendix

The Two-parameter Action

The Lagrangian of system

$$L = \frac{1}{2}[m\dot{X}^2(t) + M\dot{Y}^2(t) - \kappa(X(t) - Y(t))^2]. \tag{A.1}$$

and the propagator as

$$\begin{aligned} K(X_2Y_2, X_1Y_1; T) &= \langle X_2Y_2; T | X_1Y_1; 0\rangle \\ &= N \int D[X(t)]D[Y(t)] \exp\frac{i}{\hbar}\left\{\int_0^T dt\frac{1}{2}[m\dot{X}^2(t) - \kappa X^2(t)]\right. \\ &\quad \left. + \int_0^T dt\frac{1}{2}[M\dot{Y}^2(t) - \kappa Y^2(t) + 2X(t)Y(t)]\right\}, \end{aligned} \tag{A.2}$$

where N is a normalization constant determined so that for $\kappa = 0$

$$N = (\frac{m}{2\pi i\hbar t})^{3/2}(\frac{M}{2\pi i\hbar t})^{3/2}. \tag{A.3}$$

We shall therefore carrying out the path integral for the second particle, by using harmonic forced oscillator, Eq. (A.2) becomes

$$\begin{aligned} K(X_2Y_2, X_1Y_1; T) &= (\frac{m}{2\pi i\hbar t})^{3/2}(\frac{M}{2\pi i\hbar t})^{3/2} \\ &\quad \cdot \int D[X(t)] \exp\frac{i}{\hbar}\left\{\int_0^T dt\frac{1}{2}[m\dot{X}^2(t) - \kappa X^2(t)] \cdot \exp(S_{cl}[Y(t)])\right\}, \end{aligned} \tag{A.4}$$

where $\omega = \sqrt{\kappa/M}$ and

$$S_{cl}(Y(t)) = \frac{M\omega}{2\sin\omega t}[(Y_2^2 + Y_1^2)\cos\omega t - 2Y_2 \cdot Y_1 + \frac{2\kappa Y_2}{M\omega}\int_0^T dtX(t)\sin\omega t$$

$$+\frac{2\kappa Y_1}{M\omega}\int_0^T dtX(t)\sin\omega(T-t)-\frac{2\kappa^2}{M^2\omega^2}\int_0^T\int_0^t dtdsX(t)\cdot X(s)\sin\omega(T-t)\sin\omega s].$$

As mentioned above,we shall not be interested in the second particle. One can carry out the path integral for the second particle, thus setting $Y_2 = Y_1$ and defining the propagator for a single particle

$$K(X_2, X_1; T) = \int \delta(Y_2 - Y_1)K(X_2Y_2, X_1Y_1; T)dY_2$$

$$= (\frac{mM\omega}{(2\pi i\hbar t)(2\pi i\hbar\sin\omega t)})^{3/2}\int D[X(t)]\exp\frac{i}{\hbar}\left\{\int_0^T dt\frac{1}{2}[m\dot{X}^2(t)-\kappa X^2(t)]\right.$$

$$\times\int dY_2\exp\frac{i}{\hbar}\left[-M\omega\tan\frac{\omega}{2}T\cdot Y_2^2+\kappa\int_0^T dtX(t)(\frac{\sin\omega t+\sin\omega(T-t)}{\sin\omega T})\cdot Y_2\right]$$

$$\left.\times\exp\frac{i}{\hbar}\left[-\frac{\kappa^2}{M\omega}\int_0^T\int_0^t dtdsX(t)\cdot X(s)\frac{\sin\omega(T-t)\sin\omega s}{\sin\omega T}\right]\right\}. \qquad (A.5)$$

Now we are ready to carry out of second term in Y_2 integral, using the Gaussian formula

$$\int_{-\infty}^{\infty} dpe^{-ap^2+bp} = \sqrt{\frac{\pi}{a}}e^{\frac{b^2}{4a}}, \qquad (A.6)$$

we can write the propagator

$$K(X_2, X_1; T) = (\frac{mM\omega}{(2\pi i\hbar t)(2\pi i\hbar\sin\omega t)})^{3/2}(\frac{\pi\hbar}{iM\omega\tan\frac{\omega}{2}T})^{3/2}$$

$$\times\int D[X(t)]\exp\frac{i}{\hbar}\left\{\int_0^T dt\frac{1}{2}[m\dot{X}^2(t)-\kappa X^2(t)\right.$$

$$\left.+\frac{\kappa^2}{4M\omega\tan\frac{\omega}{2}T}\int_0^T\int_0^t dtdsX(t)\cdot X(s)(\frac{\sin\omega t+\sin\omega(T-t)}{\sin\omega T})(\frac{\sin\omega s+\sin\omega(T-s)}{\sin\omega T})\right.$$

$$-\frac{\kappa^2}{M\omega}\int_0^T\int_0^t dtdsX(t)\cdot X(s)\frac{\sin\omega(T-t)\sin\omega s}{\sin\omega T}\Bigg\}. \tag{A.7}$$

Since $\sin\omega t+\sin\omega(T-t)=2\sin\frac{\omega}{2}T\cos\frac{\omega}{2}(T-t)$, then

$$\frac{1}{\tan\frac{\omega}{2}T}(\frac{\sin\omega t+\sin\omega(T-t)}{\sin\omega T})(\frac{\sin\omega s+\sin\omega(T-s)}{\sin\omega T})$$

$$=\frac{\cos\frac{\omega}{2}(T-t)\cos\frac{\omega}{2}(T-s)}{\sin\frac{\omega}{2}T\cos\frac{\omega}{2}(T)}$$

$$=\frac{1}{\sin\omega T}[\cos\omega(T-(t+s))+\cos\omega(t-s)]. \tag{A.8}$$

Substituting equation (A.8) into equation (A.9),

$$K(X_2,X_1;T)=(\frac{m}{2\pi i\hbar T})^{3/2}\frac{1}{(2i\sin\frac{\omega}{2}T)^3}\int D[X(t)]\exp\frac{i}{\hbar}\Bigg\{\int_0^T dt\frac{1}{2}[m\dot{X}^2(t)-\kappa X^2(t)$$

$$+\frac{\kappa^2}{4M\omega\tan\frac{\omega}{2}T}\int_0^T\int_0^t dtdsX(t)\cdot X(s)[\frac{2}{4}\frac{1}{\sin\omega T}\cos\omega(T-(t+s))+\cos\omega(t-s)$$

$$-\frac{\sin\omega(T-s)\sin\omega s}{\sin\omega T}]\Bigg\}. \tag{A.9}$$

Further,

$$\frac{2}{4}(\frac{1}{\sin\omega T}\cos\omega(T-(t+s))+\cos\omega(t-s))-\frac{2\sin\omega(T-s)\sin\omega s}{2\sin\omega T}$$

$$=\frac{1}{2}\frac{\cos\omega(\frac{T}{2}-(t-s))}{\sin\frac{\omega}{2}T}, \tag{A.10}$$

substituting equation (A.10) in to equation (A.9), we have propagator

$$K(X_2,X_1;T)=(\frac{m}{2\pi i\hbar t})^{3/2}\frac{1}{(2i\sin\frac{\omega}{2}T)^3}\int D[X(t)]\exp\frac{i}{\hbar}\Bigg\{\int_0^T dt\frac{1}{2}[m\dot{X}^2(t)-\kappa X^2(t)$$

$$+\frac{\kappa^2}{2M\omega}\int_0^T\int_0^t dtdsX(t)\cdot X(s)\frac{\cos\omega(\frac{T}{2}-(t-s))}{\sin\frac{\omega}{2}T}\Bigg\}. \tag{A.11}$$

Since

$$\int_0^T \int_0^t dtdsX(t)\cdot X(s)\frac{\cos\omega(\frac{T}{2}-(t-s))}{\sin\frac{\omega}{2}T}$$
$$=\frac{1}{2}\int_0^T\int_0^T dtdsX(t)\cdot X(s)\frac{\cos\omega(\frac{T}{2}-|t-s|)}{\sin\frac{\omega}{2}T},$$

where $\omega=\sqrt{\kappa/M}$, $\kappa^2/M\omega=\kappa\omega$, then the second term in the exponential of equation (12) becomes

$$\frac{\kappa^2}{2M\omega}\int_0^T\int_0^t dtdsX(t)\cdot X(s)\frac{\cos\omega(\frac{T}{2}-(t-s))}{\sin\frac{\omega}{2}T}$$
$$=\frac{1}{4}\kappa\omega\int_0^T\int_0^T dtdsX(t)\cdot X(s)\frac{\cos\omega(\frac{T}{2}-|t-s|)}{\sin\frac{\omega}{2}T}, \qquad (A.12)$$

and

$$\int_0^T dt\frac{\cos\omega(\frac{T}{2}-|t-s|)}{\sin\frac{\omega}{2}T}=\frac{2}{\omega}, \qquad (A.13)$$

since,

$$\frac{1}{2}\int_0^T dt\kappa X^2(t)=\frac{1}{2}\kappa\frac{\omega}{2}\int_0^T\int_0^T dtds(\frac{X^2(t)+X^2(s)}{2})\frac{\cos\omega(\frac{T}{2}-|t-s|)}{\sin\frac{\omega}{2}T}. \qquad (A.14)$$

Combining equation (A.12), (A.13) and (A.14), becomes

$$K(X_2,X_1;T)=(\frac{m}{(2\pi i\hbar t)})^{3/2}\frac{1}{(2i\sin\frac{\omega}{2}T)^3}\int D[X(t)]\exp\frac{i}{\hbar}\left\{\int_0^T dt\frac{1}{2}[m\dot{X}^2(t)-\kappa X^2(t)\right.$$
$$\left.-\frac{1}{8}\kappa\omega\int_0^T\int_0^T dtds\frac{\cos\omega(\frac{T}{2}-|t-s|)}{\sin\frac{\omega}{2}T}(X(t)-X(s))^2]\right\}. \qquad (A.15)$$

Therefore, the action of two-particle model system is

$$S[X(t)]=\frac{1}{2}\int_0^T dtm\dot{X}^2(t)-\frac{1}{8}\kappa\omega\int_0^T\int_0^T dtds\frac{\cos\omega(\frac{T}{2}-|t-s|)}{\sin\frac{\omega}{2}T}(X(t)-X(s))^2.$$

Vitae

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