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นายอาจรงค์ จันทมาศ

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สาขาวิชาฟิสิกส์ ภาควิชาฟิสิกส์

คณะวิทยาศาสตร์ จุฬาลงกรณ์มหาวิทยาลัย

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DENSITY OF STATES OF ELECTRONS IN WEAK RANDOM POTENTIAL
IN TWO DIMENSIONS

Mr. Ardwarong Jantamas

A Thesis Submitted in Partial Fulfillment of the Requirements
for the Degree of Master of Science Program in Physics

Department of Physics

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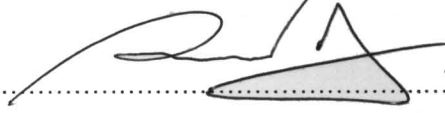
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By Mr. Ardwarong Jantamas
Field of Study Physics
Thesis Advisor Associate Professor Udomsilp Pinsook, Ph.D.


Accepted by the Faculty of Science, Chulalongkorn University in Partial
Fulfillment of the Requirements for the Master's Degree

 Dean of the Faculty of Science
(Professor Supot Hannongbua, Dr.rer.nat.)

THESIS COMMITTEE

 Chairman
(Associate Professor Mayuree Natenapit, Ph.D.)

 Thesis Advisor
(Associate Professor Udomsilp Pinsook, Ph.D.)

 Examiner
(Assistant Professor Sukkaneste Tungasmita, Ph.D.)

 External Examiner
(Assistant Professor Tanakorn Osotchan, Ph.D.)

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 เขียนที่กระจายตัวอย่างสุ่มในระบบสองมิติด้วยวิธีอินทิเกรตตามวิถีแบบแปรผัน การแปลงแบบ
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ภาควิชา ฟิสิกส์
 สาขาวิชา ฟิสิกส์
 ปีการศึกษา 2553

ลายมือชื่อนิสิต *อ.จันทมาศ*
 ลายมือชื่ออ.ที่ปรึกษาวิทยานิพนธ์หลัก *[Signature]*

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We study density of states of electrons in weak Gaussian potential model distributed randomly in the two dimensional system by the variational path integral method. The Fourier transform of Green function is separated into two parts, each part can be described as two dimensional systems with different energy range. We found the new variational method to combine two parts of the density of states with continuous and smooth slope. We observed that the frequency of the system from this method does not differ much from the other methods, and we also discussed the shifting of the Fermi-level by the impurity effect.

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CHAPTER I

Introduction

1.1 Two dimensions random systems

Although there are many two dimensional systems in physics, but our model has focused on two dimensional systems with small number of free electrons and dense defect, such as at the heterojunction systems which are heavily doped. The heterojunction is an interface layers between several different semiconductors (different band gap). We often see the heterojunction in semiconductor lasers and transistor devices (high electron mobility transistors). Many models treat the electrons moving in the heterojunction as a 2D electron gas, for example, the electrons in AlGaAs/GaAs heterojunctions [1].

A heterojunction can form the quantum well. The different band gap can confine the electrons in the conduction band, so the electron in this region can move nearly free in 2D. We can ignore the motion in a direction that is normal to the plane of the interface, so treating the problem as the 2 dimensional electron gas is a good approximation [2].

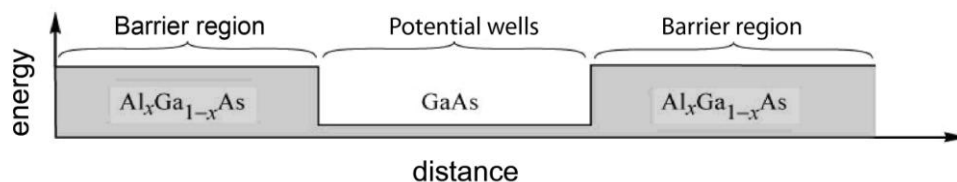


Figure 1.1 The band structure of a heterojunction that forms a quantum well.

In the real systems, the disorder effect is presented by some source of random potential. The well known example of the random media in 2 dimensions is the heavily doped charge particles randomly distributed in semiconductors. It is important because the electrical properties of semiconductor will change by doping.

1.2 Fourier transform of the potential in 2 dimensional system

The impurities in the semiconductor system can be many kinds of atoms (such as boron or phosphorus). So there are a lot of different models of the impurities' potential. Most of them are spherically symmetric so we can write the potential in terms of r . It is convenient to transform into momentum space q

$$V(\mathbf{q}) = \int d\mathbf{r} V(\mathbf{r}) e^{2\pi i \mathbf{q} \cdot \mathbf{r}} . \quad (1.1)$$

In 2D system (x-y plane) the Fourier transform can be written as

$$V(q_x, q_y) = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy V(x, y) e^{2\pi i (q_x x + q_y y)} . \quad (1.2)$$

For an isotropic system, the spherical co-ordinate is very convenient to use because the potential in physics is always spherically symmetric

$$\begin{aligned} V(q) &= \iint d\mathbf{r} V(\mathbf{r}) e^{i\mathbf{q} \cdot \mathbf{r}} \\ &= \int_{r=0}^{\infty} r dr \int_{\theta=0}^{2\pi} d\theta V(r, \theta) e^{iqr \cos(\theta)} . \end{aligned} \quad (1.3)$$

Now we are interested in the case that the potential has spherical symmetry (not depending on θ). So, $V(r, \theta) = V(r)$, and we can integrate over θ separately to obtain

$$V(q) = 2\pi \int_0^{\infty} dr V(r) J_0(qr) r , \quad (1.4)$$

When J_0 is a zeroth order Bessel function of the first kind and Eq.(1.4) is called the zeroth order Hankel transformation of $V(r)$.

1.3 The potential's model of an impurity in 2 dimensional system

The interaction between two point (static) charges in vacuum correspond to the Coulomb potential

$$V_{Coulomb}(r) = \frac{1}{4\pi\epsilon_0} \frac{Q}{r} , \quad (1.5)$$

when ϵ_0 is vacuum permittivity. If we assume that the Coulomb potential exhibits the same behavior in various dimensions, we can simply take the Fourier transform on the Coulomb potential to obtain the Coulomb potential in momentum space q in 2 dimensions,

$$V_{Coulomb2D}(q) = \frac{1}{2\epsilon_0} \frac{Q}{q}, \quad (1.6)$$

where Q is a charge of one impurity. However, when an electron moves in a random system, there are a lot of charges in the material that can interact with the electron. So the effect of impurity charge will be shielded by other atoms or ions surrounding it. The nature of charges in the semiconductor will be like a dielectric medium. Hence, the screened Coulomb potential can be used, and by considering the screening effect, the model becomes more realistic.

Now, to simplify the model, we assume that all dipoles in the dielectric medium are static so we will use the Thomas-Fermi method to approximate the value of ϵ . This method works in the case that the temperature of the system is very low. So we get

$$V_{TF}(q) = \frac{2\pi Q}{\epsilon(q + \lambda)}. \quad (1.7)$$

when ϵ is the dielectric constant and λ is a Thomas-Fermi wave vector. There are many 2D model systems studied using the Thomas-Fermi potential. [3,4]

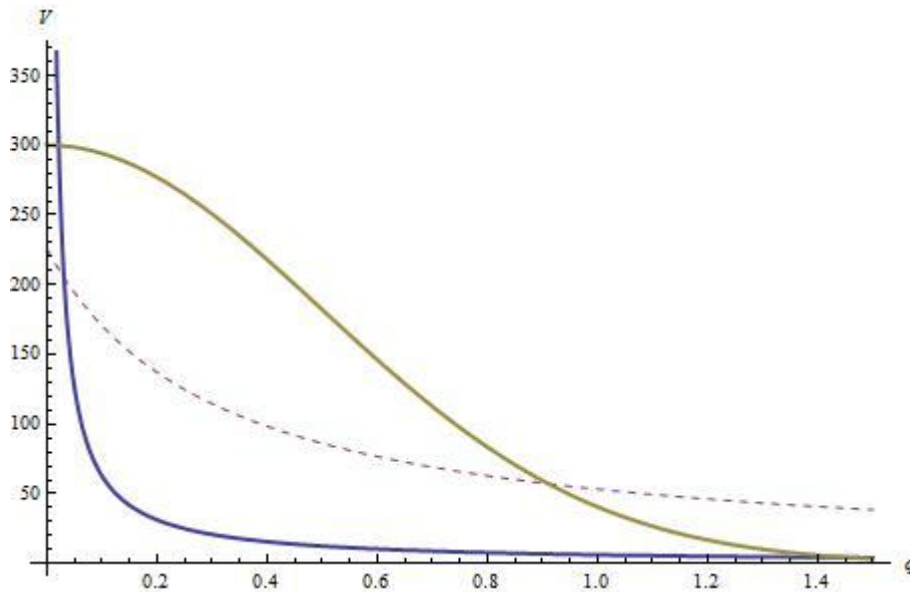


Figure 1.2 Show coulomb potential (blue thick line), is the, the Thomas-Fermi screening potential with dielectric parameter $\epsilon = 1.6$ and $\lambda = 0.01$ in arbitrary units (dashed line) and the Gaussian potential with $C = 300$ and $a = 2$ in arbitrary units (green line).

From Figure 1.2 we can see that the Thomas-Fermi potential in the momentum space do not have same behavior as the pure Coulomb potential. When $q \rightarrow 0$ the Coulomb potential tends to approach infinity but the Thomas-Fermi potential reach some value. But when $q \rightarrow \infty$, it converges to Coulomb case. We also compared the Coulomb potential and the Thomas-Fermi potential with the Gaussian potential. The Gaussian potential is our main work that we expected it can be used to represent the screening potential. We can write the Gaussian potential as

$$V_{Gaussian}(r) = C \exp(-ar^2), \quad (1.9)$$

where C is a strength of the potential, a is the parameter that is related to the shape of the potential.

1.4 The general model of semiconductors

The semiconductor is separated from the conductor and insulator by electrical property. Band gap of the semiconductor is very narrow compared to the insulator. At very low temperature, most electrons in semiconductor stay in the valence band. So at very low temperature the semiconductor have a poor conductivity. But when the temperature is higher, the electrons have more chance to jump into the conduction band. So, the semiconductor can conduct more current at high temperature. We will see this argument quantitatively, where the chance for electrons to jump into the conduction band can be approximated about $e^{\frac{-E_g}{K_B T}}$. When $K_B = 0.8617 \times 10^{-4} eV / K$, room temperature is about 300K, so $K_B T \approx 0.026 eV$. For the semiconductor, the energy gap E_g is nearly 1eV (For Si, E_g is 1.1eV at room temperature [5]). So $e^{\frac{-E_g}{K_B T}} = e^{\frac{-1.1}{0.026}} \approx 2 \times 10^{-17}$. This number seems little but one mole of matter has a lot of electrons in the order of 10^{23} . Thus, they can conduct electrical current. On the other hand, the band gap of the insulator can be 5-10eV [6]. The fraction of the transition electron is about $e^{\frac{-5}{0.026}} \approx 3 \times 10^{-84}$ implying that there is no chance for electron transition into the conduction band for insulator.

The properties of semiconductors will change if they are doped by impurities. If we add boron to the silicon by 1 boron atom to 10^5 silicon atoms, the conductivity of pure silicon

will be increased by a factor of 10^3 at room temperature [7]. The impurities can be separated into 2 groups. First is called “donor”, where the impurities have valence electrons more than valence electron of the semiconductors. So, the donor will fill electrons in the conduction band of semiconductor. The second is called “acceptor”, where the impurities have valence electrons less than the valence electrons of the semiconductors. We are now going to deal with a model that has doped with the donor and the similar argument can be applied with the acceptor.

Our general model will consider that doping is random and distributed through out the material (quite) uniformly.

If we have Si (silicon) semiconductors (4 valence electrons), and then dope it with P (phosphorus) atoms (5 valence electrons). The P atoms will substitute (replace) the Si atom as shown in figure 1.3. For simplicity, we treat the structure of P ion core (nucleus+core electrons) same as the Si atom except the positive charge and one outer electron.

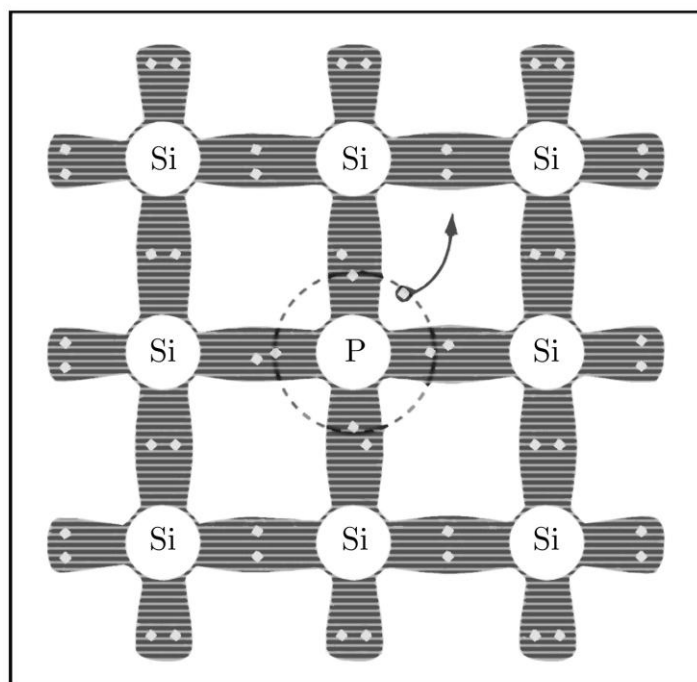


Figure 1.3 Simple view of doping P in the pure Si semiconductor.

A donor impurity will give one electron which move in the system and one positive charge of the ion core. We will focus on these electrons that came from the donors because they will affect the electronic properties of the system.

Suppose the outer electrons from donor fill in the conduction band, they can move quite freely but they also interact with

1. impurities
2. host atoms

The host semiconductor can be viewed as a dielectric medium which screen the charge of the impurity, so the conduction electrons will see the impurity charge reduced by $\frac{q}{\epsilon}$. The value of ϵ is different in various materials. The conduction electrons will interact with host atoms, where this part of interaction can make conduction electrons move easier or harder. We can describe conduction electrons with effective mass m^* . This will effect to the shape of the conduction band as shown in figure 1.4.

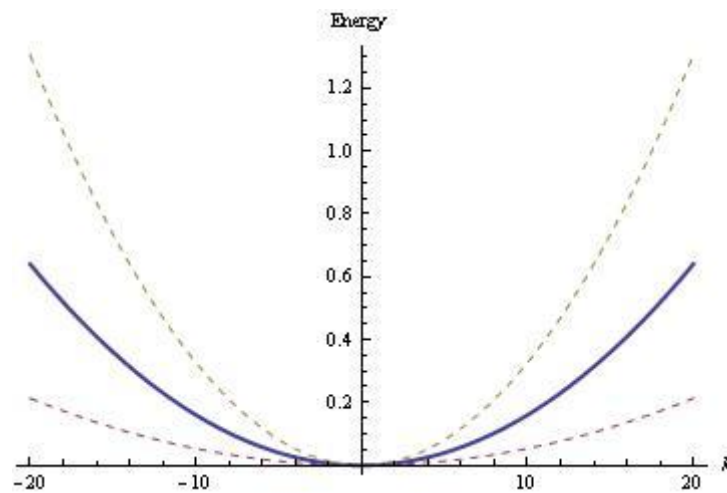


Figure 1.4 A conduction band for free electron (thick line) and conduction band when electron interacts with host atoms (dashed lines) in arbitrary units.

We treat this problem as a nearly free electron system so the shape of the conduction band will not differ much from a parabola [8]. If the conduction electron moves harder in the semiconductor, we can represent the electron's mass as the heavy electron. The heavy electron is the lower dashed line because if we look at the same momentum (same point in k-axis), the lower dashed line have lower kinetic energy $E = \frac{p^2}{2m^*}$ by higher mass. In contrast, if the conduction electron moves easier through the medium, the electron's mass will correspond with the light electron (higher dashed line).

1.5 The density of states of free electrons in 2 dimensional system

The density of states defined as the number of states $\delta\Omega(E)$ per unit volume per interval of energy ($E \rightarrow E + \delta E$)

$$D(E) = \frac{1}{V} \frac{d\Omega(E)}{dE}. \quad (1.10)$$

Now we consider a periodic system in 2 dimensional systems. We will treat the problem as a free electron moving in 2 dimension square well with length L . The equation describing a free electron in 2 dimensional systems is the free particle Schrödinger equation

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \psi(x, y) = E\psi(x, y). \quad (1.11)$$

By the separation of variable method $\psi(x, y) = X(x)Y(y)$. We quickly get the solution

$$\psi(x, y) = A \sin\left(\frac{k_x x}{2}\right) \sin\left(\frac{k_y y}{2}\right). \quad (1.12)$$

This solution satisfying the periodicity condition

$$\psi(x, y) = \psi(x + L, y) = \psi(x, y + L). \quad (1.13)$$

Where k_x and k_y are $k_x = \frac{2n_x\pi}{L} = 0, \pm \frac{2\pi}{L}, \pm \frac{4\pi}{L}, \dots$ and again with $k_y = \frac{2n_y\pi}{L}$.

By substituting the solution back into the Schrödinger equation, we will get the energy eigenvalue

$$E_k = \frac{\hbar^2}{4m} (k_x^2 + k_y^2). \quad (1.14)$$

Suppose there are a huge number of particles in order 10^{23} and they do not interact with each other. In ground state (temperature 0 K) the particles will begin filling in lowest energy and increase up to the maximum energy at

$$E_F = \frac{\hbar^2}{4m} (k_F^2). \quad (1.15)$$

which is also called the Fermi energy. This equation defined Fermi energy as the maximum energy of occupying electrons at temperature of 0 K.

In 2 dimensional k -space, two fermion states (including spin states) occupy an area of $\left(\frac{2\pi}{L}\right)^2$. The number of particle is very large so we can treat states in k -space as continuum limit. The occupying area is $4\pi k_F^2$, so total number of occupy states can be written as

$$\Omega_{total} = 2 \frac{4\pi k_F^2}{\left(\frac{2\pi}{L}\right)^2}. \quad (1.16)$$

If we are interested in some energy range $E \rightarrow E + dE$ that correspond to some range of momentum $k \rightarrow k + dk$, the occupying area in k -space is the ring $2\pi k dk$ (figure 1.5).

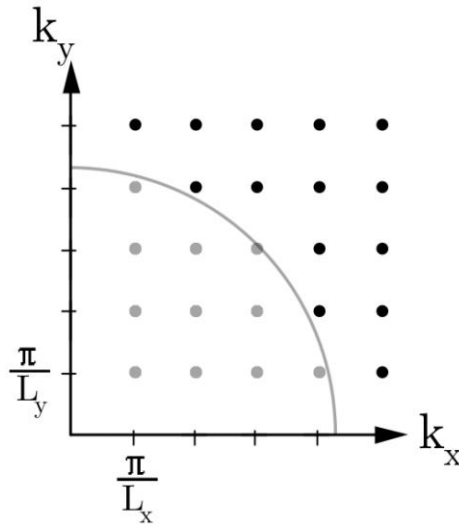


Figure 1.5 Free electron states in 2 dimensional k -space.

The total number of occupy states in that range is

$$d\Omega(E) = 2 \frac{2\pi k dk}{\left(\frac{2\pi}{L}\right)^2}. \quad (1.17)$$

And from equation 1.15, we have $k^2 = \frac{4mE}{\hbar^2}$ ($dk = \frac{4mdE}{2k\hbar^2}$). So we rewrite the number of occupy states in energy range $E \rightarrow E + dE$ as

$$d\Omega(E) = \frac{L^2}{\pi} \frac{mdE}{\hbar^2}. \quad (1.18)$$

Then we take the derivative to obtain the density of states (DOS) of free particle in 2 dimensional system (Note that there is no negative energy state for a free particle). So, the number of occupy states per interval of energy dE can be written as

$$\frac{d\Omega(E)}{dE} = \frac{mL^2 H(E)}{\pi \hbar^2} \quad (1.19)$$

where $H(E)$ is Heaviside step function. The density of states (DOS) per unit area is

$$DOS(E) = \frac{mH(E)}{\pi\hbar^2}. \quad (1.20)$$

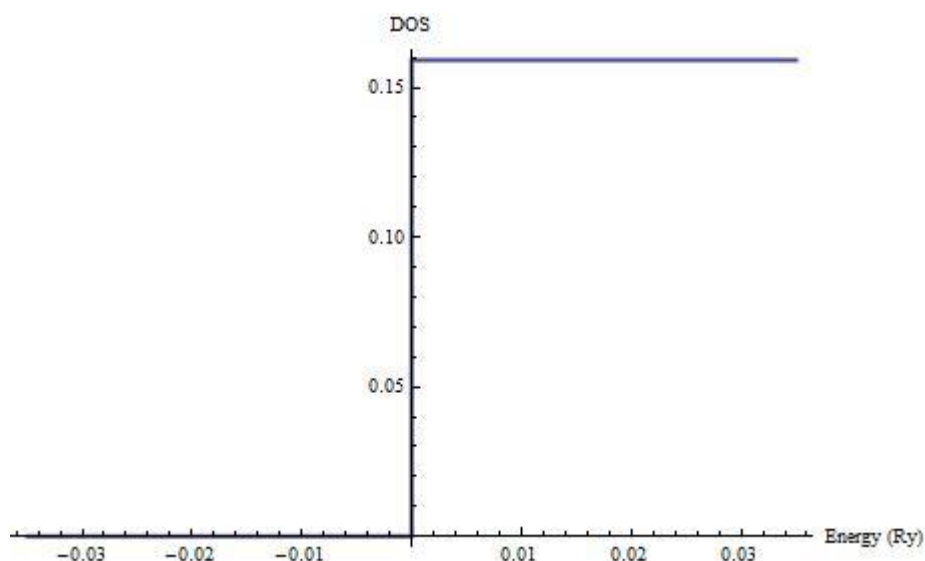


Figure 1.6 The DOS (in Rydberg units) for free electron in the conduction band.

1.6 Review of the semiconductor models

There were several approaches to obtain the density of states (DOS) of the heavily doped semiconductor. The problem is to deal with the statistical effects where there were various approximation techniques and many models to attack the problem.

In 1962, P.A. Wolff began with many electrons treatment and then showed that the electron-electron interactions can be neglected [9]. So, the nature of a single electron in the semiconductor can be treated as a particle moving in the screened fields of the impurities. This is quite the same as the general model of the semiconductor that is widely used in a lot of research and found in many text books.

In 1963, E.O. Kane proposed a theory to obtain the whole DOS in all energy range. This method was the semiclassical treatment. The semiclassical approach ignore all small fluctuations from the quantum effect if an electron wavelength is large enough compared to the changing of potential by charge impurities. The true potential $V(r)$ of the system is very complicated but this method assumed that an electron can see only the smooth potential $V_s(r)$ without any quantum contributions (Figure 1.7).

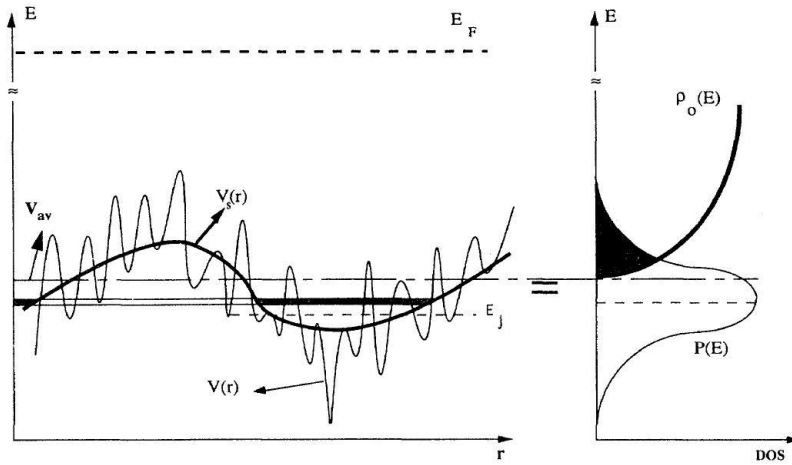


Figure 1.7 Show the actual potential ($V(r)$) and smooth potential ($V_s(r)$) that does not contain quantum fluctuation. Semiclassical approach considers states above $V_s(r)$ so the density of states is well described in the free particle region [10].

When $V(r)$ has a high (positive or negative) value, the electron will be highly localized in the narrow region so that the kinetic energy of an electron will be large. But when $V(r)$ is close to zero (quite flat) the kinetic energy is small and slowly varying with the position r . Kane's theory ignored the variation of kinetic energy with shape of $V(r)$. Thus an electron can be treated as "a free electron". Kane's method started with this equation

$$DOS(E) \propto \int_{-\infty}^E \rho_0(E' - V) P(E') dE' \quad , \quad (1.21)$$

when $\rho_0(E' - V)$ is the density of states for a free electron with energy $E' - V$. $P(E')$ is the probability distribution for states at energy E' . This method works well when energy is high $E \rightarrow \infty$. However, this density of states is quite poor to explain the tail.

In 1966, B.I. Halperin and M. Lax came up with the new approach to describe particularly the tail states [11]. They considered the deep tail (limit $E \rightarrow -\infty$) and then use the

minimum counting method to formulate the theory. They also used the variational condition to find the best of f (trial function) by maximizing the density of states

$$DOS(E, f_{\max}) = \max[DOS(E, f)],$$

$$\left(\frac{\partial}{\partial f} DOS(E, f) \right) = 0 . \quad (1.22)$$

However, the theory is not well satisfied if the energy is not deep enough or in the free particle (conduction band) region.

In 1974, a new way of variational principle was founded by Saito and Edwards [12]. They realized that there is no exact variational function that has been applied to the DOS over the entire energy range. They noticed the variational condition by maximizing the DOS was an inappropriate and tried to make the relationship between the statistical operator (connected with thermodynamics potential) and the time development operator. The final result is the variational method by maximizing $\ln(DOS(E, f))$ instead

$$\left(\frac{\partial}{\partial f} \ln(DOS(E, f)) \right) = 0 . \quad (1.23)$$

In 1975, P. Lloyd and P. R. Best proposed the new variational method by maximizing $P(E, \omega)$ function [13]. We called it the pressure function defined as

$$P(E, \omega) = \int_{-\infty}^{E_F} dE' \int_{-\infty}^{E'} dE'' DOS(E'', \omega) ,$$

$$\left(\frac{\partial P(E, \omega)}{\partial \omega} \right) = 0 \quad . \quad (1.24)$$

In 1980, Sa-yakanit and Glyde improved and applied path integral method to describe the disorder system [14]. The main idea was based on Feynman's polaron theory (1955). This method was also applied to describe effective mass in the interaction of charge Plasmon system by U. pinsook, V. Sa-yakanit and T. Bovornratanaraks (2003). In 2009, A. Thongnum, U. Pinsook, and V. Sa-yakanit extended this path integral method to obtain the density of states of the Si/Si(1-x)Ge(x) Quantum wells [15]. The application results fit to the experimental data but there are still some points that need more details of discussions.

The Fourier transform of Green function of the 2 dimensional random system is very complicated so many approximations are very important. There are several ways to estimate DOS. We are going to deal with 2 separate cases, taking $t \rightarrow \infty$ and $t \rightarrow 0$ to obtain 2 limits of Green function. Then perform Fourier transform to get 2 limits of DOS. $G(r_1, r_2; t \rightarrow \infty)$ corresponds with negative density of states $DOS(E < 0, \omega)$ that described the nature of the band tail. On the other hand, $G(r_1, r_2; t \rightarrow 0)$ corresponds with positive density of states $DOS(E > 0, \omega)$ that described free particle states. The variational principle had applied to obtain the best frequency ω of the system but DOS is still separated in 2 regions. In the real world, DOS must be continuous and smooth. The complete theory should get the whole spectrum for DOS or tell the value of the density of states at any given energy.

We have developed a new approach of getting the frequency value by using the continuous and smooth conditions. The results have been compared with the other main variational methods.

Chapter II

Review of path integral methods

Path integral is the alternative way to formulate quantum mechanics. The idea was first introduced by P. A. M. Dirac and then developed by Richard Feynman.

When we include the relativistic effect, in field theory, the path integral methods have a lot of advantages.

1. This approach is very closely fit with the scattering problem because we have the explicit form of the transition amplitude. Feynman rules can be derived very naturally.

2. Path integral quantization is the formal form, provide important descriptions and very convenient to study vacuum polarization effect [16].

3. There are a few complex systems with constraints that can only be quantized in the path integral formalism.

4. The path integral formalism can be linked between the other formalisms such as the various covariant approaches. [17]

In this research, we used the path integral methods in solid states physics.

In 1955, Feynman used variational principle with the path integral method to study the polaron problem. In short, the polaron is the hypothetical particle emerged when electrons moving in a polar crystal interact with the polarization of the lattice ions. The energy of the electrons will be lowered and its effective mass will be increased. Feynman treated the problem as that of a free electron interacting with a harmonic interaction. This theory provided accurate effective mass of an electron, mobility and optical absorption of the crystal.

In the random doping impurities in the semiconductors system, we can also use path integral methods as an alternative to calculate propagator of the electron in the doping material. Then we find DOS of the system. The DOS is the core of the solid state because we can derive a material's properties such as heat capacity, electron's mean energy, electron's velocity in the conduction band; by calculating the DOS.

2.1 The propagator by path integral

The Wave function that satisfies Schrodinger equation can be written in the form

$$\psi(\mathbf{q}, t) = \langle \mathbf{q} | \psi(t) \rangle = \langle \mathbf{q} | \hat{U}(t, t_0) | \psi(t_0) \rangle, \quad (2.1)$$

where $\hat{U}(t, t_0)$ is the well known time evolution operator. $\langle \mathbf{q} |$ is the eigenstate of position \mathbf{q} .

By using the completeness relation we can write

$$\begin{aligned} \langle \mathbf{q} | \hat{U}(t, t_0) | \psi(t_0) \rangle &= \langle \mathbf{q} | \hat{U}(t, t_0) \left(\int d\mathbf{q}_0 | \mathbf{q}_0 \rangle \langle \mathbf{q}_0 | \right) | \psi(t_0) \rangle \\ &= \int d^3 q_0 \langle \mathbf{q} | \hat{U}(t, t_0) | \mathbf{q}_0 \rangle \langle \mathbf{q}_0 | \psi(t_0) \rangle \\ &= \int d^3 q_0 K(\mathbf{q}, \mathbf{q}_0; t, t_0) \langle \mathbf{q}_0 | \psi(t_0) \rangle, \end{aligned} \quad (2.2)$$

where $K(\mathbf{q}, \mathbf{q}_0; t, t_0)$ is called the propagator. The physical meaning of propagator is the probability amplitude of a particle that starts at position \mathbf{q}_0 at time t_0 and then propagates to appear at position \mathbf{q} when the time is t when the measurement is performed. For simplicity we consider the system with only one degree of freedom. The generalization can be extended straightforwardly. So, the propagator can be written as $K(q, q_0; t, t_0) = \langle q | \hat{U}(t, t_0) | q_0 \rangle$. If we consider the propagator that makes $|q_0\rangle$ at time t_0 transition to final state $|q_f\rangle$ at time t_f

$$K(q_f, q_0; t_f, t_0) = \langle q_f | \hat{U}(t_f, t_0) | q_0 \rangle. \quad (2.3)$$

We can divide time interval to $N+1$ parts $(t_0, t_1), (t_1, t_2), \dots, (t_k, t_{k+1}), \dots, (t_N, t_f)$ and we can rewrite time evolution operator as

$$\hat{U}(t_f, t_0) = \hat{U}(t_f, t_N) \dots \hat{U}(t_1, t_0). \quad (2.4)$$

The propagator become

$$K(q_f, q_0; t_f, t_0) = \langle q_f | \hat{U}(t_f, t_0) | q_0 \rangle = \langle q_f | \prod_{k=0}^N \hat{U}(t_{k+1}, t_k) | q_0 \rangle. \quad (2.5)$$

Now the final state $\langle q_f |$ becomes $\langle q_{N+1} |$.

We can insert the completeness relation $\int dq_i | q_i \rangle \langle q_i | = 1$ between the time evolution operators

$$\langle q_f | \prod_{k=0}^N \hat{U}(t_{k+1}, t_k) | q_0 \rangle = \langle q_f | \hat{U}(t_{N+1}, t_N) \left[\int dq_N | q_N \rangle \langle q_N | \right] \hat{U}(t_N, t_{N-1}) \dots$$

$$\begin{aligned}
& \dots \left[\int dq_{k+1} |q_{k+1}\rangle \langle q_{k+1}| \right] \hat{U}(t_{k+1}, t_k) \left[\int dq_k |q_k\rangle \langle q_k| \right] \dots \\
& \dots \left[\int dq_1 |q_1\rangle \langle q_1| \right] \hat{U}(t_1, t_0) |q_0\rangle \\
& = \int dq_N dq_{N+1} \dots dq_1 \left(\prod_{k=0}^N K(q_{k+1}, q_k; t_{k+1}, t_k) \right)
\end{aligned} \tag{2.6}$$

where $K(q_{k+1}, q_k; t_{k+1}, t_k) = \langle q_{k+1} | \hat{U}(t_{k+1}, t_k) | q_k \rangle$ is the intermediate propagator.

To calculate $K(q_f, q_0; t_f, t_0)$, we have to find an explicit form of each intermediate propagator by letting

$$\hat{U}(t_{k+1}, t_k) = \exp\left[-\frac{i}{\hbar} \Delta t_k \hat{H}\right] \tag{2.7}$$

So the intermediate propagator can be written as,

$$K(q_{k+1}, q_k; t_{k+1}, t_k) = \langle q_{k+1} | \left(\exp\left[-\frac{i}{\hbar} \Delta t_k \hat{H}\right] \right) | q_k \rangle \tag{2.8}$$

By separating the Hamiltonian into $\hat{H} = \hat{T} + \hat{V}$

$$\exp\left[-\frac{i}{\hbar} \Delta t_k \hat{H}\right] = \exp\left[-\frac{i}{\hbar} \Delta t_k (\hat{T} + \hat{V})\right] \tag{2.9}$$

and using the formula*

$$e^{A+B} \approx e^A e^B e^{-\frac{1}{2}[B,A]} \tag{2.10}$$

(See appendix 1),

$$\text{We get } e^{-\frac{i}{\hbar} \Delta t_k (\hat{T} + \hat{V})} = e^{-\frac{i}{\hbar} \Delta t_k \hat{T}} e^{-\frac{i}{\hbar} \Delta t_k \hat{V}} e^{O(\Delta t_k^2)} \tag{2.11}$$

$$\begin{aligned}
\langle q_{k+1} | \left(\exp\left[-\frac{i}{\hbar} \Delta t_k \hat{H}\right] \right) | q_k \rangle &= \langle q_{k+1} | e^{-\frac{i}{\hbar} \Delta t_k \hat{T}} e^{-\frac{i}{\hbar} \Delta t_k \hat{V}} e^{O(\Delta t_k^2)} | q_k \rangle \\
&= \langle q_{k+1} | e^{-\frac{i}{\hbar} \Delta t_k \hat{T}} \left(\int dq_i |q_i\rangle \langle q_i| \right) e^{-\frac{i}{\hbar} \Delta t_k \hat{V}} | q_k \rangle e^{O(\Delta t_k^2)} \\
&= \int dq_i \langle q_{k+1} | e^{-\frac{i}{\hbar} \Delta t_k \hat{T}} | q_i \rangle \langle q_i | e^{-\frac{i}{\hbar} \Delta t_k \hat{V}} | q_k \rangle e^{O(\Delta t_k^2)}
\end{aligned} \tag{2.12}$$

We consider the first term (kinetic) in the integral

$$\begin{aligned}
\langle q_{k+1} | \exp\left(-\frac{i}{\hbar} \Delta t_k \hat{T}\right) | q_i \rangle &= \langle q_{k+1} | \exp\left(-\frac{i}{\hbar} \Delta t_k \hat{T}\right) \left(\int dp_k |p_k\rangle \langle p_k| \right) | q_i \rangle \\
&= \int dp_k \langle q_{k+1} | \exp\left(-\frac{i}{\hbar} \Delta t_k \hat{T}\right) | p_k \rangle \langle p_k | q_i \rangle
\end{aligned}$$

$$= \int dp'_k \exp\left(-\frac{i}{\hbar} \Delta t_k T(p_k)\right) \langle q_{k+1} | p_k \rangle \langle p_k | q_i \rangle \quad (2.13)$$

And we find that

$$\begin{aligned} \langle q_{k+1} | p_k \rangle &= \frac{1}{\sqrt{2\pi\hbar}} \exp\left(\frac{ip_k q_{k+1}}{\hbar}\right) \text{ and } \langle p_k | q_i \rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left(-\frac{ip_k q_i}{\hbar}\right) \\ &= \int dp_k \exp\left(-\frac{i}{\hbar} \Delta t_k T(p_k)\right) \frac{1}{\sqrt{2\pi\hbar}} \exp\left(\frac{ip_k q_{k+1}}{\hbar}\right) \frac{1}{\sqrt{2\pi\hbar}} \exp\left(-\frac{ip_k q_i}{\hbar}\right) \\ &= \int dp_k \frac{1}{2\pi\hbar} \exp\left(-\frac{i}{\hbar} \Delta t_k T(p_k)\right) \exp\left(\frac{ip_k (q_{k+1} - q_i)}{\hbar}\right) \end{aligned} \quad (2.14)$$

We turn to the second term (potential) in the integral

$$\begin{aligned} \langle q_i | \exp\left(-\frac{i}{\hbar} \Delta t_k (\hat{V})\right) | q_k \rangle &= \exp\left(-\frac{i}{\hbar} \Delta t_k V(q_k)\right) \langle q_i | q_k \rangle \\ &= \exp\left(-\frac{i}{\hbar} \Delta t_k V(q_k)\right) \delta(q_i - q_k) \end{aligned} \quad (2.15)$$

Then

$$\begin{aligned} K(q_{k+1}, q_k; t_{k+1}, t_k) &= \langle q_{k+1} | \left[\exp\left[-\frac{i}{\hbar} \Delta t_k \hat{H}\right] \right] | q_k \rangle \\ &= \int dp_k \int dq_i \frac{1}{2\pi\hbar} \delta(q_i - q_k) \exp\left(-\frac{i}{\hbar} \Delta t_k (T(p_k) + V(q_k)) + \right. \\ &\quad \left. + \frac{ip_k (q_{k+1} - q_i)}{\hbar} + O(\Delta t_k^2)\right) \end{aligned}$$

We get $T(p_k) + V(q_k) = H(p_k, q_k)$

$$\begin{aligned} &= \int dp_k \frac{1}{2\pi\hbar} \exp\left(-\frac{i}{\hbar} \Delta t_k H(p_k, q_k) + \frac{ip_k (q_{k+1} - q_k)}{\hbar} + O(\Delta t_k^2)\right) \\ &= \int dp_k \frac{1}{2\pi\hbar} \exp\left(\frac{i}{\hbar} \Delta t_k \left(\frac{p_k (q_{k+1} - q_k)}{\Delta t_k} - H(p_k, q_k)\right) + O(\Delta t_k^2)\right) \end{aligned} \quad (2.16)$$

This is the intermediate propagator and the total propagator can be written in terms of it as

$$\begin{aligned} K(q_f, q_0; t_f, t_0) &= \int dq_N dq_{N+1} \dots dq_1 \left(\prod_{k=0}^N K(q_{k+1}, q_k; t_{k+1}, t_k) \right) \\ &= \int \prod_{k=1}^N \frac{dp_k dq_k}{(2\pi\hbar)^N} \int \frac{dp_0}{2\pi\hbar} \exp\left(\sum_{k=0}^N \frac{i}{\hbar} \Delta t_k \left(\frac{p_k (q_{k+1} - q_k)}{\Delta t_k} - H(p_k, q_k)\right) + O(\Delta t_k^2)\right) \end{aligned} \quad (2.17)$$

Letting $N \rightarrow \infty$ and $\Delta t_k \rightarrow 0$ we can see that p and q are the functions of continuous time such that $p(t)$ and $q(t)$, at some particular time t_k , are $p(t_k) \equiv p_k$ and $q(t_k) \equiv q_k$. We replace discrete summation in the exponential term by integral.

$$\begin{aligned} & \lim_{N \rightarrow \infty} \left(\sum_{k=0}^N \frac{i}{\hbar} \Delta t_k \left(\frac{p_k(q_{k+1} - q_k)}{\Delta t_k} - H(p_k, q_k) \right) + O(\Delta t_k^2) \right) \\ & , \\ & = \int_{t_0}^{t_f} \frac{i}{\hbar} dt \left(p(t) \frac{dq(t)}{dt} - H(p(t), q(t)) \right) \end{aligned} \quad (2.18)$$

when $N \rightarrow \infty$ we introduce the notation

$$\mathbf{D}p \mathbf{D}q \equiv \lim_{N \rightarrow \infty} \frac{1}{(2\pi\hbar)^{N+1}} \left(\prod_{k=1}^N dp_k dq_k \right) dp_0 \quad (2.19)$$

Now we obtain the total propagator

$$K(q_f, q_0; t_f, t_0) = \int_{q_0}^{q_f} \mathbf{D}p \mathbf{D}q \exp \left(\int_{t_0}^{t_f} \frac{i}{\hbar} dt (p\dot{q} - H(p, q)) \right) \quad (2.20)$$

This is the general form of the propagator for any form of the Hamiltonian. However, in the real physical system, the Hamiltonian always depends on the square of the momentum $H(p_k, q_k) = \frac{p_k^2}{2m} + V(q_k)$. Nonetheless, we will continue to work on simplifying the general propagator (2.20) to get more specific result to be more widely used in physics. For now, let us put the Hamiltonian in to the intermediate propagator (2.16).

$$K(q_{k+1}, q_k; t_{k+1}, t_k) = \int dp_k \frac{1}{2\pi\hbar} \exp \left(\frac{i}{\hbar} \Delta t_k \left(\frac{p_k(q_{k+1} - q_k)}{\Delta t_k} - \frac{p_k^2}{2m} - V(q_k) \right) + O(\Delta t_k^2) \right) \quad (2.21)$$

We can perform this integral over p_k by using a form of Gaussian integral.

$$K(q_{k+1}, q_k; t_{k+1}, t_k) = \sqrt{\frac{m}{2\pi i \hbar \Delta t_k}} \exp \left(\frac{i}{\hbar} \Delta t_k \left(\frac{m(q_{k+1} - q_k)^2}{2\Delta t_k^2} - V(q_k) \right) + O(\Delta t_k^2) \right) \quad (2.22)$$

Then, we substitute this expression into 2.17 and taking $N \rightarrow \infty$, $\Delta t_k \rightarrow 0$ and using this relation

$$\lim_{N \rightarrow \infty} \sum_{k=0}^N \left(\frac{m(q_{k+1} - q_k)^2}{2\Delta t_k^2} - V(q_k) \right) \Delta t_k = \int_{t_0}^{t_f} dt \left(\frac{m\ddot{q}}{2} - V(q) \right) = S. \quad (2.23)$$

Finally, we have the total propagator

$$K(q_f, q_0; t_f, t_0) = \int_{q(t_0)=q_0}^{q(t_f)=q_f} \mathbf{D}q \exp \left(\frac{iS}{\hbar} \right), \quad (2.24)$$

$$\text{with } \mathbf{D}q = \frac{1}{\sqrt{2\pi i \hbar m^{-1} \Delta t_0}} \prod_{k=1}^{\infty} \frac{dq_k}{\sqrt{2\pi i \hbar m^{-1} \Delta t_k}}. \quad (2.25)$$

This is the most important formula that we used through out our research.

In the discrete limit

$$K(q_f, q_0; t_f, t_0) \propto \sum_{\text{all path}} \exp\left(\frac{iS}{\hbar}\right) = \exp\left(\frac{iS_1}{\hbar}\right) + \exp\left(\frac{iS_2}{\hbar}\right) + \dots + \exp\left(\frac{iS_N}{\hbar}\right), \quad (2.26)$$

where S_N correspond to one path. This is why we call path integral.

2.2 The classical limit of the propagators.

How classical path differ from quantum path? The propagator (2.26) can interpret the classical behavior of particles and this will fill our point of view of quantum behavior. This view comes from R.P. Feynman [18]. In classical mechanics, the explicit form of any Lagrangian will lead to the specific equation of motion through the famous Euler-Lagrange equation. If we restrict our system by imposing initial conditions $x(t_0)$, $\dot{x}(t_0)$, the system will evolve in time by itself and correspond to some particular path. Now we are in a position to say that we have clear an explicit path of a particle.

In quantum mechanics, when we look at the equation (2.26), the propagator is depending on the sum of the quantity $\exp\left(\frac{iS}{\hbar}\right)$ along all paths in space (The word ‘‘all paths’’ was interpreted from $\int_{q(t_0)=q_0}^{q(t_f)=q_f} \mathbf{D}q$).

Little changing in path may cause a little changing action. In classical limit, $\hbar \ll S$ so we can say that in this limit $\hbar \rightarrow 0$ [19]. If we look at the quantity $\exp\left(\frac{iS}{\hbar}\right)$ as sum of sine and cosine function, when $\hbar \rightarrow 0$, this quantity correspond to the very high frequency for sinusoidal function. But in high frequency limit, we can see by simple mathematics that the summing of sine (or cosine) function will tend to be zero (because the violent changing of phase will contain some phase that differs by π radian). Thus, almost every path will have destructive interference and cancel out each other. So, when $\hbar \rightarrow 0$ most path will not emerge, except when the action is at the minimum value, because $dS = 0$ at minimum point. Hence, little changing in path will make no changing in action. Therefore, summing

neighboring path ($dS \neq 0$) will make the quantity $\exp\left(\frac{iS}{\hbar}\right)$ destructive of each other and the path that makes $dS = 0$ will appear as a classical path. In figure 2.1, the thick line is the actual path that makes action has minimum value and dotted lines around it are the neighboring paths.

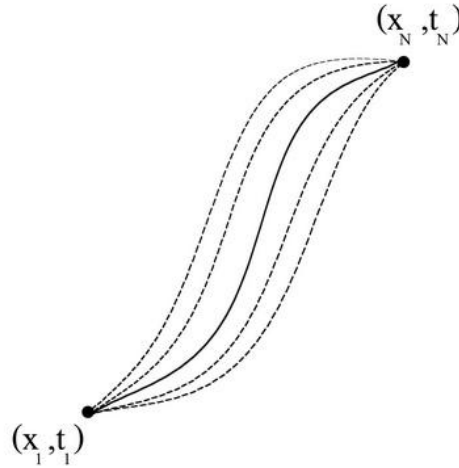


Figure 2.1 The solid line is the classic path. The dashed lines are the variation of paths that tend to cancel with one another [18].

In the quantum view, action is very small $S \approx \hbar$, so the neighboring paths will make a significant change in $\exp\left(\frac{iS}{\hbar}\right)$ and there is no cancellation. In other word, the contribution comes from all possible paths. At this point we have shown something that joints the classical and quantum mechanics.

In our research, we will use (2.24) and (2.25) to find the electron propagator in two dimensional systems.

CHAPTER III

Review of variational path integral method

We will now deal with the random problem. We first assume the impurities are completely random, such as heavily doping a semiconductor. For simplicity, we ignore the lattice structure of the semiconductor. The impurities are possibly found in all points in two-dimensional space. The idea is acceptable because electronics properties are of the macroscopic scale. Many electrons in the band contribute to conductivity of the semiconductor. Therefore, the structure of atoms in the semiconductor is not quite affected.

3.1 Calculation of an average electron propagator in Gaussian random potential

We suppose the impurities are distributed in the semiconductor system with the position $\{\mathbf{r}_i\}$. The action of an electron interacting with one configuration impurities is $S(\{\mathbf{r}_i\})$. The propagator of the particular configuration of the impurities can be written as

$$\mathbf{G}(\{\mathbf{r}_i\}; t) = \int \mathbf{D}\mathbf{r}(\tau) \exp\left[\frac{i}{\hbar} S(\{\mathbf{r}_i\})\right], \quad (3.1)$$

where $\mathbf{G}(\{\mathbf{r}_i\}; t)$ is Green function with particular configuration impurities. So, the average Green function ($G(r_1, r_2; t)$) over all possible configurations is

$$G(r_1, r_2; t) = \int d(\{\mathbf{r}_i\}) P(\{\mathbf{r}_i\}) \mathbf{G}(\{\mathbf{r}_i\}; t), \quad (3.2)$$

where $P(\{\mathbf{r}_i\})$ is the probability to find the impurities in the configuration $\{\mathbf{r}_i\}$. Our main problem in this chapter is finding the average Green function $G(r_1, r_2; t)$. We assume the impurities are equally found in two-dimensional space (see appendix D). Then we apply this assumption to the average Green function and the result reads [20]

$$G(r_1, r_2; t) = \int \mathbf{D}\mathbf{r}(\tau) \exp\left[\frac{i}{\hbar} \int_0^t d\tau \frac{m}{2} \dot{\mathbf{r}}^2(\tau) + n \int d\mathbf{R} \left[\exp\left(-\frac{i}{\hbar} \int_0^t d\tau v(\mathbf{r}(\tau) - \mathbf{R})\right) - 1 \right]\right], \quad (3.3)$$

when n is impurities per unit area. If we are interested in the weak scattering process $v \rightarrow 0$ (or $|v| \ll 1$ Ry), we can expand the exponential term in the second term

$$\exp\left(-\frac{i}{\hbar} \int_0^t d\tau v(\mathbf{r}(\tau) - \mathbf{R})\right) \approx 1 - \frac{1}{2\hbar^2} \int_0^t d\tau \int_0^t d\sigma v(\mathbf{r}(\tau) - \mathbf{R})v(\mathbf{r}(\sigma) - \mathbf{R}). \quad (3.4)$$

Now the average Green function becomes

$$\begin{aligned} G(r_1, r_2; t) &= \int \mathbf{D}\mathbf{r}(\tau) \exp\left[\frac{i}{\hbar} \int_0^t d\tau \frac{m}{2} \dot{\mathbf{r}}^2(\tau) + n \int d\mathbf{R} \left[-\frac{1}{2\hbar^2} \int_0^t d\tau \int_0^t d\sigma v(\mathbf{r}(\tau) - \mathbf{R})v(\mathbf{r}(\sigma) - \mathbf{R})\right]\right] \\ &= \int \mathbf{D}\mathbf{r}(\tau) \exp\left[\frac{i}{\hbar} \int_0^t d\tau \frac{m}{2} \dot{\mathbf{r}}^2(\tau) - \frac{n^2}{2\hbar^2} \int_0^t d\tau \int_0^t d\sigma W(\mathbf{r}(\tau) - \mathbf{r}(\sigma))\right], \end{aligned} \quad (3.5)$$

where W is the correlation function defined as $W(\mathbf{r}(\tau) - \mathbf{r}(\sigma)) = \int v(\mathbf{r}(\tau) - \mathbf{R})v(\mathbf{r}(\sigma) - \mathbf{R})d\mathbf{R}$. If we restrict our problem to the Gaussian potential $V_{Gaussian}(\mathbf{r} - \mathbf{R}) = b \exp(-a(\mathbf{r} - \mathbf{R})^2)$, we will obtain the Gaussian correlation function as

$$W(\mathbf{r}(\tau) - \mathbf{r}(\sigma)) = \frac{C'}{\pi L^2} \exp\left[-\frac{(\mathbf{r}(\tau) - \mathbf{r}(\sigma))^2}{L^2}\right], \quad (3.6)$$

where C' and L are the parameters we can adjust and C' is the interaction strength and L is the correlation length. We can see the problem is too complicated to be solved because we do not know the exact position of vector $\mathbf{r}(\tau)$. Hence, the harmonic trial is implemented to solve the problem. Now, to simplify, we will write the average Green function in a short form

$$G(r_1, r_2; t) = \int \mathbf{D}\mathbf{r} \exp\left(\frac{iS}{\hbar}\right), \quad (3.7)$$

$$\text{where } S = \int_0^t d\tau \frac{m}{2} \dot{\mathbf{r}}^2(\tau) + \frac{n^2 i}{2\hbar} \int_0^t d\tau \int_0^t d\sigma W(\mathbf{r}(\tau) - \mathbf{r}(\sigma)). \quad (3.8)$$

The first term in (3.8) is the kinetic term and the second term is the interaction term, where η is the strength of the scattering potential.

3.2 The harmonic trial action

The average Green function $G(r_1, r_2; t)$ of an electron can be written as

$$G(r_1, r_2; t) = \int \mathbf{D}r \exp\left(\frac{iS}{\hbar}\right) = \left(\int \mathbf{D}r \exp\left(\frac{iS_0}{\hbar}\right) \right) \times \exp\left[\frac{i}{\hbar}(S - S_0(\omega))\right], \quad (3.9)$$

Where $S_0 = \int_0^t d\tau \left(\frac{m}{2} \dot{x}^2(\tau) - \frac{m\omega^2}{2t} \int_0^t d\sigma |x(\tau) - x(\sigma)|^2 \right)$ is the simple harmonic action and ω is the frequency of the system. We use the simple harmonic action as the trial action because we know the exact solution of such system. Then we apply the identity [21]

$$\langle X \rangle_{S_0} = \frac{\int \mathbf{D}r \exp\left(\frac{iS_0}{\hbar}\right) X}{\int \mathbf{D}r \exp\left(\frac{iS_0}{\hbar}\right)}. \quad (3.10)$$

This is the statistical average of quantity X over S_0 , where S_0 is the harmonic oscillator action which we use it as the trial action. The variational parameter (ω) is the frequency of the oscillators in the system.

If we need the average of $\exp\left[\frac{i}{\hbar}(S - S_0(\omega))\right]$, we can write it as

$$\left\langle \exp\left[\frac{i}{\hbar}(S - S_0(\omega))\right] \right\rangle_{S_0} = \frac{\int \mathbf{D}r \exp\left(\frac{iS_0}{\hbar}\right) \exp\left[\frac{i}{\hbar}(S - S_0(\omega))\right]}{\int \mathbf{D}r \exp\left(\frac{iS_0}{\hbar}\right)}. \quad (3.11)$$

This is a very important formula because we can use it to find average Green function $G(r_1, r_2; t)$ of an electron. Now we can rewrite (3.9) as

$$G(r_1, r_2; t) = \int \mathbf{D}r \exp\left(\frac{iS}{\hbar}\right) = \left(\int \mathbf{D}r \exp\left(\frac{iS_0}{\hbar}\right) \right) \times \left\langle \exp\left[\frac{i}{\hbar}(S - S_0(\omega))\right] \right\rangle_{S_0}. \quad (3.12)$$

To move forward, we quote the Kubo cumulant expansion [22]

$$\langle e^X \rangle = \exp\left[\langle X \rangle + \frac{1}{2!} (\langle X^2 \rangle - \langle X \rangle^2) + \frac{1}{3!} (\langle X^3 \rangle - 3\langle X \rangle [\langle X^2 \rangle - \langle X \rangle^2] - \langle X \rangle^3) \dots \right] \quad (3.13)$$

If we choose the frequency to make the trial action close enough to our interested action, we can keep only the first order to obtain the approximate average Green function

$$G(r_1, r_2; t) \approx G_1(r_1, r_2; t) = \left(\int \mathbf{D}r \exp\left(\frac{iS_0}{\hbar}\right) \right) \times \exp\left[\frac{i}{\hbar} \langle S - S_0(\omega) \rangle_{S_0}\right]. \quad (3.14)$$

To obtain the approximate Green function $G_1(r_1, r_2; t)$, we separate our problem to find 3 parts

1. $\left(\int \mathbf{D}r \exp\left(\frac{iS_0}{\hbar}\right) \right)$
2. $\langle S_0(\omega) \rangle_{S_0}$
3. $\langle S \rangle_{S_0}$.

3.3 The propagator of the simple harmonic action for the random system

For the first part, what we will find is the propagator of the simple harmonic action

$$K_0(r_2, r_1; t, \omega) = \left(\int \mathbf{D}r \exp\left(\frac{iS_0}{\hbar}\right) \right), \quad (3.15)$$

where the action is $S_0 = \int_0^t d\tau \left(\frac{m}{2} \dot{x}^2(\tau) - \frac{m\omega^2}{2t} \int_0^t d\sigma |x(\tau) - x(\sigma)|^2 \right)$. We will now try to obtain a more general action in quadratic form and then specify the result to the simple harmonic action later.

The quadratic action can obtain from the Lagrangian in this form

$$L(x, \dot{x}; t) = a(t)x^2 + b(t)x\dot{x} + c(t)\dot{x}^2 + d(t)x + e(t)\dot{x} + f(t). \quad (3.16)$$

In our problem (simple harmonic), the coefficient $b(t)$ and $e(t)$ is obviously vanished, and then we split the particle's path into two parts

$$x(t) = \bar{x}(t) + y(t), \quad (3.17)$$

$$\dot{x}(t) = \dot{\bar{x}}(t) + \dot{y}(t), \quad (3.18)$$

where $\bar{x}(t)$ is the classical path that make $dS=0$, and $y(t)$ is the disturbed path. Then we expand the Lagrangian around the classical path $\bar{x}(t)$ with Taylor series. All higher terms after the square term will vanish because the original Lagrangian has only the quadratic term.

$$L(x, \dot{x}; t) = L(\bar{x}, \dot{\bar{x}}; t) + \left. \frac{\partial L}{\partial x} \right|_{\bar{x}} y + \left. \frac{\partial L}{\partial \dot{x}} \right|_{\dot{\bar{x}}} \dot{y} + \frac{1}{2} \left(\left. \frac{\partial^2 L}{\partial x^2} \right|_{\bar{x}} y^2 + 2 \left. \frac{\partial^2 L}{\partial x \partial \dot{x}} \right|_{\bar{x}} y \dot{y} + \left. \frac{\partial^2 L}{\partial \dot{x}^2} \right|_{\dot{\bar{x}}} \dot{y}^2 \right). \quad (3.19)$$

We take partial derivative on the Lagrangian to get

$$\frac{\partial^2 L}{\partial x^2} = 2a(t), \quad \frac{\partial^2 L}{\partial x \partial \dot{x}} = b(t), \quad \frac{\partial^2 L}{\partial \dot{x}^2} = 2c(t). \quad (3.20)$$

So the action of this Lagrangian can be written as

$$S = \int_0^t L(x, \dot{x}; t) d\tau = \int_0^T L(\bar{x}, \dot{\bar{x}}; t) dt + \int_0^T \left(\frac{\partial L}{\partial x} \Big|_{\bar{x}} y + \frac{\partial L}{\partial \dot{x}} \Big|_{\dot{\bar{x}}} \dot{y} \right) dt + \int_0^T (a(t)y^2 + b(t)y\dot{y} + c(t)\dot{y}^2) dt. \quad (3.21)$$

The second term will vanish by using integral by part [23]. The action is finally written as

$$S = S_{cl} + \int_0^T (a(t)y^2 + b(t)y\dot{y} + c(t)\dot{y}^2) dt. \quad (3.22)$$

So, the propagator reads

$$K_0(x_2, T; x_1, 0) = \left(\int \mathbf{D}r \exp\left(\frac{iS_0}{\hbar}\right) \right) = e^{\frac{i}{\hbar}S_{cl}} \times \int \mathbf{D}y \exp\left(\frac{i}{\hbar} \int_0^T (a(t)y^2 + b(t)y\dot{y} + c(t)\dot{y}^2) dt\right) = A(T) e^{\frac{i}{\hbar}S_{cl}}. \quad (3.23)$$

Now, we focus on our simple harmonic action. The classical action for simple harmonic action is (appendix C)

$$S_{cl} = \frac{m\omega}{4} \cot\left(\frac{1}{2}\omega t\right) |X_2 - X_1|^2. \quad (3.24)$$

We will try to find $A(T)$ to complete the propagator.

We consider the propagator

$$H(x_2, T; x_1, 0; y) = \left(\int \mathbf{D}r \exp\left(\frac{i}{\hbar} \left[\int_0^t d\tau \left(\frac{m}{2} \dot{r}^2(\tau) - \frac{m\omega^2}{2} |r(\tau) - y|^2 \right) \right] \right) \right). \quad (3.25)$$

It is the simple harmonic propagator with the parameter y . If $y=0$, H will be reduced to the normal simple harmonic propagator. We will now prove the identity

$$\int H(x_2, T; x_1, 0; y) dy = \sqrt{\frac{2\pi\hbar}{im\omega^2 t}} K_0(r_2, r_1; t, \omega), \quad (3.26)$$

Where $K_0(r_2, r_1; t, \omega) = \left(\int \mathbf{D}r \exp\left(\frac{iS_0}{\hbar}\right) \right)$ is the simple harmonic propagator in our problem. This is proven easily because we can perform the integral over y to both sides of the equation (3.25)

$$\begin{aligned} \int H(x_2, T; x_1, 0; y) dy &= \int dy \left(\int \mathbf{D}r \exp\left(\frac{i}{\hbar} \left[\int_0^t d\tau \left(\frac{m}{2} \dot{r}^2(\tau) - \frac{m\omega^2}{2} |r(\tau) - y|^2 \right) \right] \right) \right) \\ &= \int \mathbf{D}r \left(\left(\exp\left(\frac{i}{\hbar} \left[\int_0^t d\tau \frac{m}{2} \dot{r}^2(\tau) \right] \right) \right) \times \int dy \exp\left(\frac{i}{\hbar} \left[\int_0^t d\tau \left(-\frac{m\omega^2}{2} |r(\tau) - y|^2 \right) \right] \right) \right). \end{aligned} \quad (3.27)$$

Doing nothing with the kinetic term and focus on the potential term

$$\begin{aligned} &\int dy \exp\left(\frac{i}{\hbar} \left[\int_0^t d\tau \left(-\frac{m\omega^2}{2} |r(\tau) - y|^2 \right) \right] \right) \\ &= \int dy \exp\left(-\frac{m\omega^2}{2} \frac{i}{\hbar} \left[\int_0^t d\tau (r^2(\tau) - 2r(\tau)y + y^2) \right] \right) \\ &= \exp\left(-\frac{m\omega^2}{2} \frac{i}{\hbar} \left[\int_0^t d\tau r^2(\tau) \right] \right) \int dy \exp\left(-\frac{m\omega^2}{2} \frac{i}{\hbar} \left[-\int_0^t d\tau 2r(\tau)y + ty^2 \right] \right). \end{aligned} \quad (3.28)$$

The second term is the Gaussian integral over y ,

$$\begin{aligned} &\int dy \exp\left(-\frac{m\omega^2}{2} \frac{i}{\hbar} \left[\left(\sqrt{t}y - \frac{\int_0^t d\tau r(\tau)}{\sqrt{t}} \right)^2 - \frac{\left(\int_0^t d\tau r(\tau) \right)^2}{t} \right] \right) \\ &= \sqrt{\frac{\pi 2\hbar}{im\omega^2 t}} \exp\left(-\frac{m\omega^2}{2} \frac{i}{\hbar} \frac{\left(\int_0^t d\tau r(\tau) \right)^2}{t} \right). \end{aligned} \quad (3.29)$$

The total result becomes

$$\begin{aligned} &\int H(x_2, T; x_1, 0; y) dy \\ &= \sqrt{\frac{\pi 2\hbar}{im\omega^2 t}} \int \mathbf{D}r \left(\left(\left(\exp\left(\frac{i}{\hbar} \left[\int_0^t d\tau \frac{m}{2} \dot{r}^2(\tau) - \frac{m\omega^2}{2} \left[\int_0^t d\tau r^2(\tau) \right] - \frac{m\omega^2}{2} \frac{\left(\int_0^t d\tau r(\tau) \right)^2}{t} \right) \right] \right) \right) \right) \end{aligned}$$

$$= \sqrt{\frac{\pi 2\hbar}{im\omega^2 t}} K_0. \quad (3.30)$$

If we are interested in two-dimensional system, the equation (3.30) will become

$$\int H(x_2, T; x_1, 0; y) dy = \frac{2\pi\hbar}{im\omega^2 t} K_0. \quad (3.31)$$

Then, we perform integral $\int dr$ to both sides of the equation (3.30)

$$\int K_0 dr = \left(\frac{2\pi\hbar}{im\omega^2 t} \right)^{-1} \int dr \int dy H(x_2, T; x_1, 0; y). \quad (3.32)$$

We see $\int K_0 dr = \int A(T) e^{\frac{i}{\hbar} S_{cl}} dr = A(T) \int e^{\frac{i}{\hbar} S_{cl}} dr = A(T) V_0$, where $V_0 = \int e^{\frac{i}{\hbar} S_{cl}} dr$ is the term we are not interested in. Here, we quote the result $\int dr \int dy H(x_2, T; x_1, 0; y) = \left(2i \sin\left(\frac{1}{2} \omega t\right) \right)^{-2} V_0$ [22]. Then we get

$$\int K_0 dr = \left(\frac{2\pi\hbar}{im\omega^2 t} \right)^{-1} \left(2i \sin\left(\frac{1}{2} \omega t\right) \right)^{-2} V_0 = A(T) V_0, \quad (3.33)$$

$$A(T) = \left(\frac{m\omega^2 t}{8i\pi\hbar} \right) \left(\frac{1}{\sin\left(\frac{\omega t}{2}\right)} \right)^2. \quad (3.34)$$

The result is

$$\begin{aligned} K_0(r_2, r_1; t, \omega) &= \left(\int \mathbf{D}r \exp\left(\frac{iS_0}{\hbar}\right) \right) \\ &= \left(\frac{m\omega^2 t}{8i\pi\hbar} \right) \left(\frac{1}{\sin\left(\frac{\omega t}{2}\right)} \right)^2 \exp\left(\frac{i}{\hbar} \left(\frac{m\omega}{4} \cot\left(\frac{1}{2} \omega t\right) |X_2 - X_1|^2 \right)\right). \end{aligned} \quad (3.35)$$

Since the impurity in our system is spread randomly, we apply the translational invariant to our result and get

$$K_0(r_2, r_1; t, \omega) = \left(\int \mathbf{D}r \exp\left(\frac{iS_0}{\hbar}\right) \right) = \left(\frac{m\omega^2 t}{8i\pi\hbar} \right) \left(\frac{1}{\sin\left(\frac{\omega t}{2}\right)} \right)^2. \quad (3.36)$$

3.4 The average of simple harmonic action

The second part we will find is the average of the simple harmonic action

$$\langle S_0(\omega) \rangle_{s_0} = \left\langle \int_0^t d\tau \frac{1}{2} m \dot{r}^2(\tau) \right\rangle_{s_0} - \left\langle \frac{m\omega^2}{2t} \int_0^t d\tau \int_0^t d\sigma [r(\tau) - r(\sigma)]^2 \right\rangle_{s_0} . \quad (3.37)$$

The kinetic term from the simple harmonic action will cancel the kinetic term of the Gaussian action. Therefore, we can just find the average on the second term that contributes

$$-\frac{m\omega^2}{2t} \left\langle \int_0^t d\tau \int_0^t d\sigma [r(\tau) - r(\sigma)]^2 \right\rangle$$

The problem involves with the average value of $\langle r(\tau)r(\sigma) \rangle$.

If S' is the action of harmonic oscillator with the driven force $\mathbf{F}(\tau)$, and S is the simple harmonic oscillator, we can write

$$S' = S_0 + \int d\tau \mathbf{F}(\tau) \cdot \mathbf{r}(\tau) . \quad (3.38)$$

We can write the propagator of S' and S_0 as

$$\left(\int \mathbf{D}r \exp\left(\frac{iS'}{\hbar}\right) \right) = A'(T) \exp\left(\frac{i}{\hbar} S'_{cl}\right) \quad (3.39)$$

$$\left(\int \mathbf{D}r \exp\left(\frac{iS_0}{\hbar}\right) \right) = A(T) \exp\left(\frac{i}{\hbar} S_{0cl}\right) \quad (3.40)$$

It is easy to show that $A'(T)$ from S' is equal to $A(T)$ from S_0 . We will, again, use this equation

$$\langle X \rangle_{s_0} = \frac{\int \mathbf{D}r \exp\left(\frac{iS_0}{\hbar}\right) X}{\int \mathbf{D}r \exp\left(\frac{iS_0}{\hbar}\right)} . \quad (3.41)$$

We then substitute $X = \exp\left(\frac{i}{\hbar} \int d\tau \mathbf{F}(\tau) \cdot \mathbf{r}(\tau)\right)$ in this average equation (3.41), and then we obtain

$$\left\langle \exp\left(\frac{i}{\hbar} \int d\tau \mathbf{F}(\tau) \cdot \mathbf{r}(\tau)\right) \right\rangle_{S_0} = \frac{\int \mathbf{D}\mathbf{r} \exp\left(\frac{iS'}{\hbar}\right)}{\int \mathbf{D}\mathbf{r} \exp\left(\frac{iS_0}{\hbar}\right)} = \exp\left(\frac{i}{\hbar} [S'_{cl} - S_{0cl}]\right). \quad (3.42)$$

Then, we take the functional derivative with respect to $\mathbf{F}(\tau)$ on the left hand side of (3.42) by using this formula

$$\frac{\delta \exp\left(\int d\tau q(\tau) f(\tau)\right)}{\delta q(\tau)} = f(\tau) \exp\left(\int d\tau q(\tau) f(\tau)\right), \quad (3.43)$$

We get

$$\frac{\delta \left\langle \exp\left(\frac{i}{\hbar} \int d\tau \mathbf{F}(\tau) \cdot \mathbf{r}(\tau)\right) \right\rangle_{S_0}}{\delta \mathbf{F}(\tau)} = \frac{i}{\hbar} \times \left\langle \mathbf{r}(\tau) \exp\left(\frac{i}{\hbar} \int d\tau \mathbf{F}(\tau) \cdot \mathbf{r}(\tau)\right) \right\rangle_{S_0}. \quad (3.44)$$

We also take the functional derivative with respect to $\mathbf{F}(\tau)$ on the right hand side too. We know that $\mathbf{F}(\tau)$ is in the $S'_{cl}(\mathbf{F}(\tau), \mathbf{F}(\sigma))$ (as we can see in (3.38)), so we get

$$\frac{\delta \exp\left(\frac{i}{\hbar} [S'_{cl} - S_{0cl}]\right)}{\delta \mathbf{F}(\tau)} = \frac{i}{\hbar} \frac{\delta S'_{cl}}{\delta \mathbf{F}(\tau)} \exp\left(\frac{i}{\hbar} [S'_{cl} - S_{0cl}]\right). \quad (3.45)$$

Then we let the LHS=RHS

$$\left\langle \mathbf{r}(\tau) \exp\left(\frac{i}{\hbar} \int d\tau \mathbf{F}(\tau) \cdot \mathbf{r}(\tau)\right) \right\rangle_{S_0} = \frac{\delta S'_{cl}}{\delta \mathbf{F}(\tau)} \exp\left(\frac{i}{\hbar} [S'_{cl} - S_{0cl}]\right). \quad (3.46)$$

We take the value at $\mathbf{F}(\tau) = 0$ on both sides. It is obvious that when $\mathbf{F}(\tau) = 0$, we have $S'_{cl} = S_{0cl}$, and we now obtain the very important formula

$$\langle \mathbf{r}(\tau) \rangle_{S_0} = \left. \frac{\delta S'_{cl}}{\delta \mathbf{F}(\tau)} \right|_{\mathbf{F}=0}. \quad (3.47)$$

We can then rewrite (3.46) as

$$\left\langle \mathbf{r}(\tau) \exp\left(\frac{i}{\hbar} \int d\sigma \mathbf{F}(\sigma) \cdot \mathbf{r}(\sigma)\right) \right\rangle_{S_0} = \frac{\delta S'_{cl}}{\delta \mathbf{F}(\tau)} \exp\left(\frac{i}{\hbar} [S'_{cl} - S_{0cl}]\right). \quad (3.48)$$

Changing the dummy variable in the integral, we take functional derivative with respect to $\mathbf{F}(\tau)$ on (3.39)

$$\begin{aligned} & \frac{i}{\hbar} \left\langle \mathbf{r}(\tau) \cdot \mathbf{r}(\sigma) \exp \left(\frac{i}{\hbar} \int d\sigma \mathbf{F}(\sigma) \cdot \mathbf{r}(\sigma) \right) \right\rangle_{S_0} \\ &= \frac{\delta^2 S'_{cl}}{\delta F(\sigma) \delta F(\tau)} \exp \left(\frac{i}{\hbar} [S'_{cl} - S_{0cl}] \right) + \frac{i}{\hbar} \frac{\delta S'_{cl} \delta S'_{cl}}{\delta F(\sigma) \delta F(\tau)} \exp \left(\frac{i}{\hbar} [S'_{cl} - S_{0cl}] \right). \end{aligned} \quad (3.49)$$

Again, we set the value at $\mathbf{F}(\tau) = 0$ on both sides of (3.49), and we have

$$\langle \mathbf{r}(\tau) \cdot \mathbf{r}(\sigma) \rangle_{S_0} = \frac{\hbar}{i} \left(\frac{\delta^2 S'_{cl}}{\delta F(\sigma) \delta F(\tau)} + \frac{i}{\hbar} \frac{\delta S'_{cl} \delta S'_{cl}}{\delta F(\sigma) \delta F(\tau)} \right) \Big|_{F=0}. \quad (3.50)$$

Our particular form of action S'_{cl} makes these quantities vanish

$$\frac{\delta^2 S'_{cl}}{\delta F(\tau) \delta F(\tau)} = \frac{\delta^2 S'_{cl}}{\delta F(\sigma) \delta F(\sigma)} = 0. \quad (3.51)$$

After performing the integration (3.37), we get [23]

$$\begin{aligned} \langle S_0(\omega) \rangle_{S_0} &= \frac{3}{2} i \hbar \left(\frac{1}{2} \omega t \cot \left(\frac{1}{2} \omega t \right) - 1 \right) \\ &+ \frac{1}{2} m \left(\frac{1}{2} \omega t \cos \left(\frac{1}{2} \omega t \right) - \left[\frac{1}{2} \omega t \csc \left(\frac{1}{2} \omega t \right) \right]^2 \right) \frac{(r_2 - r_1)^2}{2t}. \end{aligned} \quad (3.52)$$

If the system is completely random, we can impose the translational symmetry on $\langle S_0(\omega) \rangle_{S_0}$. The quantity in the translational symmetric system must not depend on $(r_2 - r_1)$. So, we simply set $(r_2 - r_1) = 0$ and then we get

$$\langle S_0(\omega) \rangle_{S_0} = \frac{3}{2} i \hbar \left(\frac{1}{2} \omega t \cot \left(\frac{1}{2} \omega t \right) - 1 \right). \quad (3.53)$$

3.5 The average of Gaussian action

The third part that we will find is the average of Gaussian action

$$\langle S \rangle_{S_0} = \frac{i}{2\hbar} \left\langle \int_0^t d\tau \int_0^t d\sigma W(r(\tau) - r(\sigma)) \right\rangle_{S_0}. \quad (3.54)$$

If we restrict the problem to the Gaussian potential, the correlation function will become

$$W(r(\tau) - r(\sigma)) = \frac{C'}{\pi L^2} \exp\left[-\frac{(r(\tau) - r(\sigma))^2}{L^2}\right]. \quad (3.55)$$

It is convenient to work with the correlation function in k-space

$$W(k) = \int d\mathbf{r} W(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} = C \exp\left[-\frac{L^2 k^2}{4}\right]. \quad (3.56)$$

We will substitute (3.56) in (3.54)

$$\begin{aligned} & \frac{i}{2\hbar} \left\langle \int_0^t d\tau \int_0^t d\sigma \frac{C'}{\pi L^2} \exp\left[-\frac{(r(\tau) - r(\sigma))^2}{L^2}\right] \right\rangle_{s_0} \\ &= \frac{i}{2\hbar} \int_0^t d\tau \int_0^t d\sigma \int d^2\mathbf{k} \frac{1}{(2\pi)^2} W(k) \langle e^{-i\mathbf{k}\cdot(\mathbf{r}(\tau) - \mathbf{r}(\sigma))} \rangle. \end{aligned} \quad (3.57)$$

Again we quote the Kubo expansion and keep only the second order term

$$\begin{aligned} \langle e^{-i\mathbf{k}\cdot(\mathbf{r}(\tau) - \mathbf{r}(\sigma))} \rangle &\approx \exp\left[\langle -i\mathbf{k}\cdot(\mathbf{r}(\tau) - \mathbf{r}(\sigma)) \rangle \right. \\ &\quad \left. + \frac{1}{2!} \left(\frac{1}{2} \langle (-i\mathbf{k}\cdot(\mathbf{r}(\tau) - \mathbf{r}(\sigma)))^2 \rangle - \langle -i\mathbf{k}\cdot(\mathbf{r}(\tau) - \mathbf{r}(\sigma)) \rangle^2 \right) \right] \\ &= \exp\left[-i\mathbf{k}\cdot\langle(\mathbf{r}(\tau) - \mathbf{r}(\sigma))\rangle \right. \\ &\quad \left. + \frac{1}{2!} \left(\frac{k^2}{2} \langle(\mathbf{r}(\tau) - \mathbf{r}(\sigma))^2\rangle - \langle(\mathbf{r}(\tau) - \mathbf{r}(\sigma))\rangle^2 \right) \right]. \end{aligned} \quad (3.58)$$

Then we integrate over k_x in (3.57) by using this integration formula

$$\int_{-\infty}^{\infty} dk_x \exp\left[-(iak_x + bk_x^2)\right] = \sqrt{\frac{\pi}{b}} \exp\left[-\frac{a^2}{4b}\right], \quad (3.59)$$

where $a = \langle(\mathbf{r}(\tau) - \mathbf{r}(\sigma))\rangle_x$, $b = \frac{1}{2} \left(\frac{1}{2} \langle(\mathbf{r}(\tau) - \mathbf{r}(\sigma))^2\rangle - \langle(\mathbf{r}(\tau) - \mathbf{r}(\sigma))\rangle^2 \right) + \frac{L^2}{4}$.

In two-dimensional system, we get

$$\int d^2\mathbf{k} W(k) \left\langle e^{-i\mathbf{k}\cdot(\mathbf{r}(\tau)-\mathbf{r}(\sigma))} \right\rangle = C \frac{\pi}{b} \exp\left[-\frac{a^2}{2b}\right]. \quad (3.60)$$

So, we now have

$$\langle S \rangle_{s_0} = \frac{iC}{8\pi\hbar} \int_0^t d\tau \int_0^t d\sigma \frac{1}{b} \exp\left[-\frac{a^2}{2b}\right], \quad (3.61)$$

where a and b can be calculated by using equation (3.47) and (3.50) [24]. The results are

$$a = \langle (\mathbf{r}(\tau) - \mathbf{r}(\sigma)) \rangle = \frac{\sin\left(\frac{1}{2}\omega(\tau - \sigma)\right) \cos\left(\frac{1}{2}\omega(1 - (\tau + \sigma))\right)}{\sin\left(\frac{1}{2}\omega t\right)} (\mathbf{r}_2 - \mathbf{r}_1) \quad (3.62)$$

$$b = \frac{i\hbar}{m\omega} \left(\frac{\sin\left(\frac{1}{2}\omega(\tau - \sigma)\right) \sin\left(\frac{1}{2}\omega(t - (\tau - \sigma))\right)}{\sin\left(\frac{1}{2}\omega t\right)} \right) + \frac{L^2}{4}. \quad (3.63)$$

Now, we simply impose the translational symmetric condition $(r_2 - r_1) = 0$. So, we get $a = 0$ and

$$\langle S \rangle_{s_0} = \frac{iC}{8\pi\hbar} \int_0^t d\tau \int_0^t d\sigma \frac{1}{b} \quad (3.64)$$

If we collect all expressions, we can write the total Green function as

$$\begin{aligned} G_1(r_1, r_2; t) &= \left(\int \mathbf{D}r \exp\left(\frac{iS_0}{\hbar}\right) \right) \times \exp\left[\frac{i}{\hbar} \langle S - S_0(\omega) \rangle_{s_0}\right] \\ &= \left(\frac{m\omega^2 t}{8i\pi\hbar}\right) \left(\frac{1}{\sin\left(\frac{\omega t}{2}\right)}\right)^2 \times \exp\left(\frac{i}{\hbar} \left(\frac{3}{2}i\hbar \left(\frac{1}{2}\omega t \cot\left(\frac{1}{2}\omega t\right) - 1\right) - \frac{iC}{8\pi\hbar} \int_0^t d\tau \int_0^t d\sigma \frac{1}{b}\right)\right) \end{aligned} \quad (3.65)$$

3.6 The total Green function and the density of states in the Gaussian random potential in two-dimensional system

The density of states (DOS) is the Fourier Transform of the Green function [25].

$$DOS(E, \omega) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} G_1(r_1, r_2; t) e^{\frac{iEt}{\hbar}} \quad (3.66)$$

This equation is too complicated to be solved analytically and there are many ways to approximate the density of states (DOS). We will look back at the equation

$$\begin{aligned} \langle S \rangle_{s_0} &= \frac{i}{2\hbar} \int_0^t d\tau \int_0^t d\sigma \int d^2\mathbf{k} \frac{1}{(2\pi)^2} W(k) \langle e^{-i\mathbf{k} \cdot (\mathbf{r}(\tau) - \mathbf{r}(\sigma))} \rangle \\ &= \frac{it}{2\hbar} \int_0^t d\sigma \int d^2\mathbf{k} \frac{1}{(2\pi)^2} W(k) \exp \left[-\frac{i\hbar\mathbf{k}^2}{m\omega} \left(\frac{\sin\left(\frac{1}{2}\omega\sigma\right)\sin\left(\frac{1}{2}\omega(t-\sigma)\right)}{\sin\left(\frac{1}{2}\omega t\right)} \right) \right] \end{aligned} \quad (3.67)$$

We will separate the Green function and also the DOS in 2 limits.

1. When $t \rightarrow 0$, it is corresponding to short time interaction. The situation connected with the high energy region $E \gg 0$ [26]. The argument in the exponential reaches zero and we can expand it as follows

$$\frac{it}{2\hbar} \int_0^t d\sigma \int d^2\mathbf{k} \frac{1}{(2\pi)^2} W(k) \left[1 - \frac{i\hbar\mathbf{k}^2}{m\omega} \left(\frac{\sin\left(\frac{1}{2}\omega\sigma\right)\sin\left(\frac{1}{2}\omega(t-\sigma)\right)}{\sin\left(\frac{1}{2}\omega t\right)} \right) \right]$$

Then we can work out the exponential term to be

$$\begin{aligned} e^{\frac{i}{\hbar}\langle S \rangle_{s_0}} &= \exp \left(-\frac{t}{2\hbar^2} \int_0^t d\sigma \int d^2\mathbf{k} \frac{1}{(2\pi)^2} W(k) \right) \\ &\times \exp \left(-\frac{t}{2\hbar^2} \int_0^t d\sigma \int d^2\mathbf{k} \frac{1}{(2\pi)^2} W(k) \left[-\frac{i\hbar\mathbf{k}^2}{m\omega} \left(\frac{\sin\left(\frac{1}{2}\omega\sigma\right)\sin\left(\frac{1}{2}\omega(t-\sigma)\right)}{\sin\left(\frac{1}{2}\omega t\right)} \right) \right] \right). \end{aligned} \quad (3.68)$$

We then expand the second term and obtain the approximate $e^{\frac{i}{\hbar}\langle S \rangle_{s_0}}$

$$e^{\frac{i}{\hbar}\langle S \rangle_{s_0}} \approx \exp \left(-\frac{t^2}{2\hbar^2} \int d^2\mathbf{k} \frac{1}{(2\pi)^2} W(k) \right)$$

$$\times \left[1 - \frac{t}{2\hbar^2} \int_0^t d\sigma \int d^2\mathbf{k} \frac{1}{(2\pi)^2} W(k) \left[-\frac{i\hbar\mathbf{k}^2}{m\omega} \left(\frac{\sin\left(\frac{1}{2}\omega\sigma\right)\sin\left(\frac{1}{2}\omega(t-\sigma)\right)}{\sin\left(\frac{1}{2}\omega t\right)} \right) \right] \right]. \quad (3.69)$$

Then we perform the integral over σ and take limit $t \rightarrow 0$

$$\int_0^t d\sigma \left(\frac{\sin\left(\frac{1}{2}\omega\sigma\right)\sin\left(\frac{1}{2}\omega(t-\sigma)\right)}{\sin\left(\frac{1}{2}\omega t\right)} \right) \approx \frac{\omega t^2}{12} \quad (3.70)$$

We get

$$e^{\frac{i}{\hbar}\langle S \rangle_{s_0}} \approx \exp\left(-\frac{t^2\gamma^2}{2\hbar^2}\right) \left(1 + \frac{it^3}{24m\hbar} F^2 \right), \quad (3.71)$$

where $\gamma^2 = \int d^2\mathbf{k} \frac{1}{(2\pi)^2} W(k)$, and $F^2 = \int d^2\mathbf{k} \frac{\mathbf{k}^2}{(2\pi)^2} W(k)$. We have the Green function in the form of

$$G_1(r_1, r_2; t \rightarrow 0) = \left(\frac{m}{2i\pi\hbar t} \right) \times \exp\left(-\frac{\gamma^2 t^2}{2\hbar^2}\right) \times \left[1 + \frac{F^2 it^3}{24m\hbar} \right]. \quad (3.72)$$

We take the Fourier transform and we get the DOS for the positive energy region.

$$DOS_+(E > 0, \omega) = \frac{m}{\pi\hbar^2} \left[\frac{1}{2} \left(1 + \operatorname{erf}\left(\frac{E}{\sqrt{2}\gamma}\right) \right) - \frac{\hbar^2 F^2}{24\sqrt{2\pi m}\gamma^3} \left(1 - \frac{E^2}{\gamma^2} \right) \exp\left(-\frac{E}{2\gamma^2}\right) \right] \quad (3.73)$$

2. Now consider $t \rightarrow \infty$ that corresponds to low energy. This limit represents the states in the band tail region [26]. The quantum effect is important for the short range potential so we can consider the electron to be staying in the system long enough to take long time limit

$$\langle S \rangle_{s_0} \approx \frac{it}{2\hbar} \int_0^t d\sigma \int d^2\mathbf{k} \frac{1}{(2\pi)^2} W(k) \exp\left[-\frac{i\hbar\mathbf{k}^2 \sin\left(\frac{1}{2}\omega\sigma\right)}{m\omega} \right]. \quad (3.74)$$

After we perform the integral and collect all terms, we quickly get

$$G_1(r_1, r_2; t \rightarrow \infty) = \left(\frac{im\omega^2 t}{2\pi\hbar e} \right) \times \exp\left(-\frac{i\omega t}{2} - \frac{Q^2 t^2}{2\hbar^2} \right), \quad (3.75)$$

and we get the density of states for the negative energy region

$$DOS_-(E < 0, \omega) = \frac{m}{e\pi\hbar^2} \left[\frac{(\hbar\omega)^2 (\hbar\omega/2 - E)}{\sqrt{2\pi} Q^3(\omega)} \exp\left(-\frac{(\hbar\omega/2 - E)^2}{2Q^2(\omega)} \right) \right], \quad (3.76)$$

where $\gamma^2 = \frac{C}{\pi L^2}$, (3.77)

$$F^2 = \frac{4C}{\pi L^4}, \quad (3.78)$$

$$Q^2(\omega) = \frac{\gamma^2 \omega}{\omega + 2\hbar/mL^2}. \quad (3.79)$$

Next chapter we will use the variational methods to obtain the frequency (ω) that joins the $DOS_+(E > 0, \omega)$ with $DOS_-(E < 0, \omega)$.

CHAPTER IV

Results and discussion

We have obtained the density of states (DOS) by path integral method. First, the semiclassical DOS well describes the positive energy region by

$$DOS_+(E > 0) = \frac{m}{\pi\hbar^2} \left[\frac{1}{2} \left(1 + \operatorname{erf} \left(\frac{E}{\sqrt{2}\gamma} \right) \right) - \frac{\hbar^2 F^2}{24\sqrt{2\pi m}\gamma^3} \left(1 - \frac{E^2}{\gamma^2} \right) \exp \left(-\frac{E}{2\gamma^2} \right) \right]. \quad (4.1)$$

When there is no interaction, the semiclassical DOS will reduce to free particle states

$DOS_{free}(E > 0) = \frac{m}{\pi\hbar^2}$. Secondly, DOS describes the negative energy or tail states as

$$DOS_-(E < 0, \omega) = \frac{m}{e\pi\hbar^2} \left[\frac{(\hbar\omega)^2 (\hbar\omega/2 - E)}{\sqrt{2\pi}Q^3(\omega)} \exp \left(-\frac{(\hbar\omega/2 - E)^2}{2Q^2(\omega)} \right) \right]. \quad (4.2)$$

However, the frequency ω needs to be determined. We will use the variational methods to find the ω . For simplicity and reducing the number in the calculations, we will write all variable in the Rydberg unit.

4.1 Density of states from maximized DOS method.

We can assume that the frequency ω (variational parameter) depends on energy $\omega = \omega(E)$. At ground state, the system will be in minimum total energy. The minimum total energy is the stable states for the electron. The total energy of the electron can be written as

$$E_{tot} = \int DOS(E', \omega) E' dE'. \quad (4.3)$$

The total energy of the bound states can be found by summation all number of states multiplied by energy in bound states [27]. Since all energy in bound states are negative, if we want to get the minimum total energy, the density of states must have maximum positive value. So, we have to find function $\omega(E)$ that maximize DOS.

We use the numerical calculation by plotting the DOS with the frequency at some specific energy value. Figure 4.1 is an example of plotting for $E=0$. We pick the ω that

maximizes DOS, and in the case of $E=0$, we obtain $\omega = 0.043$. We then repeat the process to get the $\omega(E)$ that maximizes DOS.

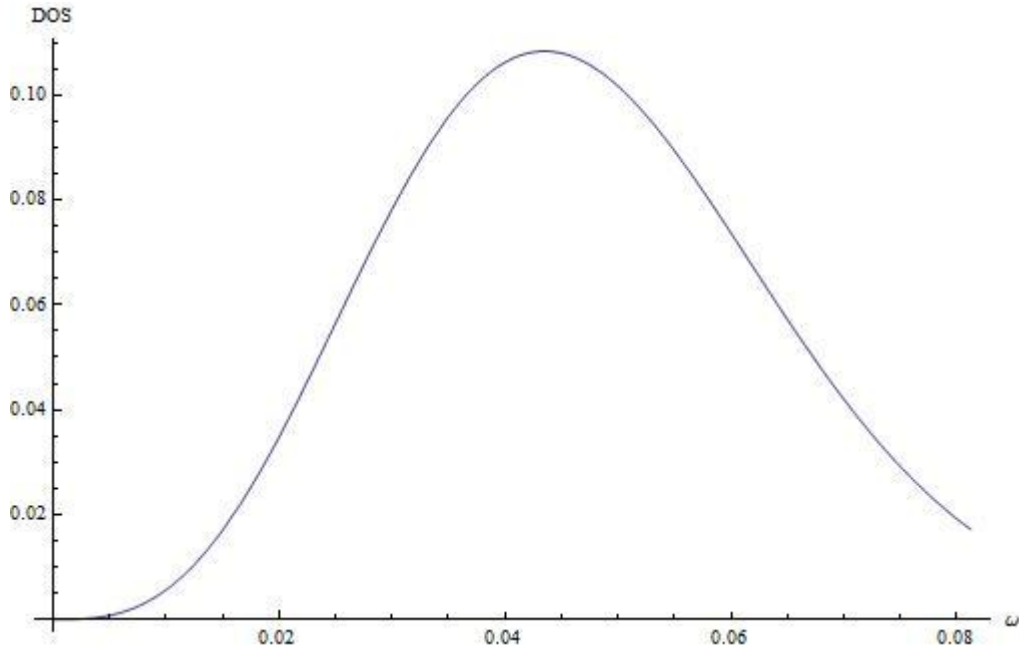


Figure 4.1 Show DOS (4.2) in Rydberg unit with $C = 5$, $L = 100$, $E = 0$, and the frequency in Rydberg units.

For $C = 5$, $L = 100$, we can find the frequency $\omega = \omega(E)$ that maximizes the DOS,

$$\omega(E) \approx 0.043 + (1.26)E + (16.64)E^2 + (73.61)E^3. \quad (4.4)$$

We choose the polynomial fit because it is easy to analyze and the results are not different from the exponential fit in this energy range.

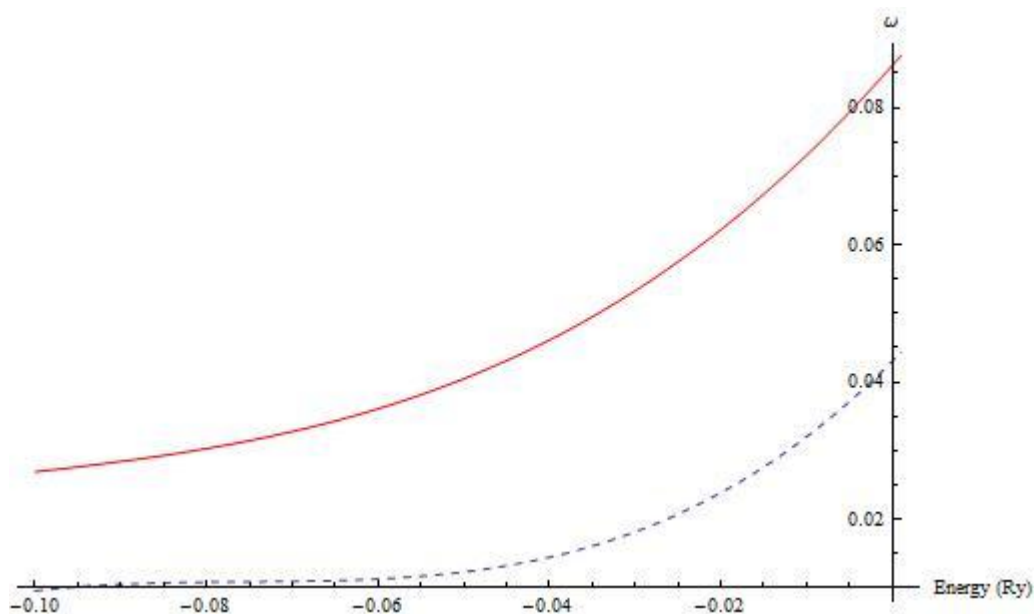


Figure 4.2 The frequency $\omega(E)$ (4.4) in Rydberg units from maximized DOS method for various correlation length (L), $L = 100$ (dashed line) and $L = 50$ (thick line).

Considering the DOS, if we plot the DOS by this method, we will see that the tail is very close to the semiclassical result as in figure 4.3. However, there remain some problems with the whole DOS as we shall see in the figure 4.4. The negative density of states (4.2) with the frequency we obtained from maximized DOS method is not connected smoothly with the positive region.

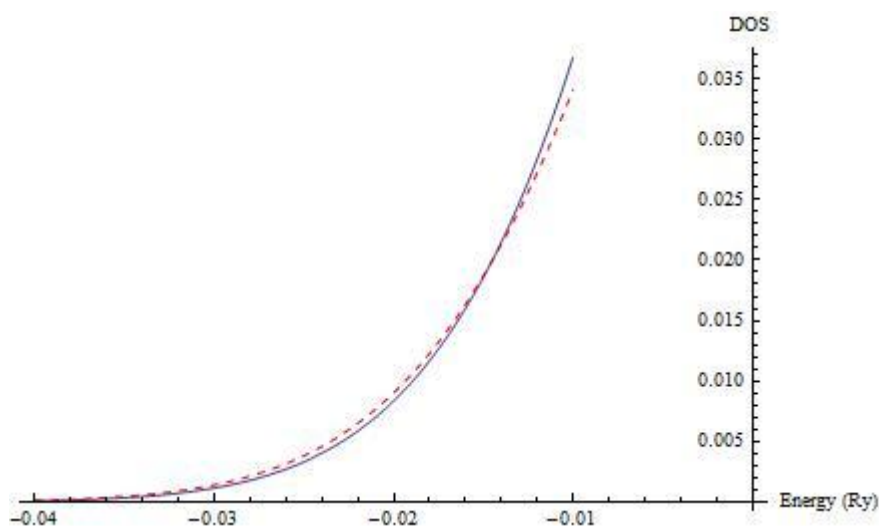


Figure 4.3 The DOS (4.2) obtained from maximized DOS (blue line), and DOS (4.1) from semiclassical approximation (red line) in Rydberg units.

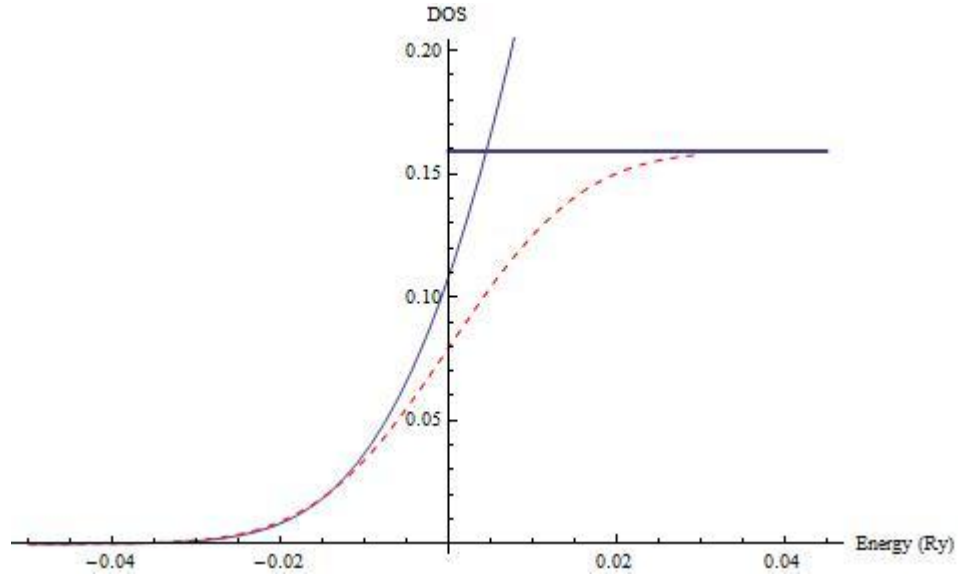


Figure 4.4 The DOS (4.2) with the frequency from maximized DOS method (blue thin line) , the DOS (4.1) of semiclassical approximation (red dashed line) and free particle DOS (1.19) (thick line) in Rydberg unit.

4.2 Density of states from minimum total energy method.

We are now interested in the total energy of the system and try to find the frequency to minimize it directly. We want the system have the minimum total energy. We will then compare the result with the maximized DOS method.

When the system is filled only in bound states, we can find E_{tot} by

$$E_{tot} = \int_{-\infty}^E D_-(E', \omega) E' dE' \quad (4.5)$$

$$E_{tot}(E, \omega) = \frac{m\omega^2 \left\{ -\sqrt{\pi} + \frac{\sqrt{2}e^{-\frac{(-2E+\hbar\omega)^2}{8q^2}} E}{q} + \sqrt{\pi} \operatorname{Erf} \left(\frac{-2E + \hbar\omega}{2\sqrt{2}q} \right) \right\}}{2e\pi^{3/2}} \quad (4.6)$$

Taking the derivative and find the frequency that satisfy the condition

$$\frac{\partial E_{tot}(E', \omega)}{\partial \omega} = 0. \quad (4.7)$$

For specific C and L , we perform contour plot of E (x-axis) and ω (y-axis). With the middle line having the zero value, we map this line with the polynomial function to obtain $\omega(E) \approx a_0 + a_1E + a_2E^2 + a_3E^3$. We keep only a_3E^3 because in our interested energy range, a_3E^3 is in the order 10^{-4} which is much lesser than the first term. Figure 4.5 is the contour plot between the frequency $\omega(E)$ (y-axis) and the energy (x-axis). The isolated curve (bottom left) in the picture is frequency equation.

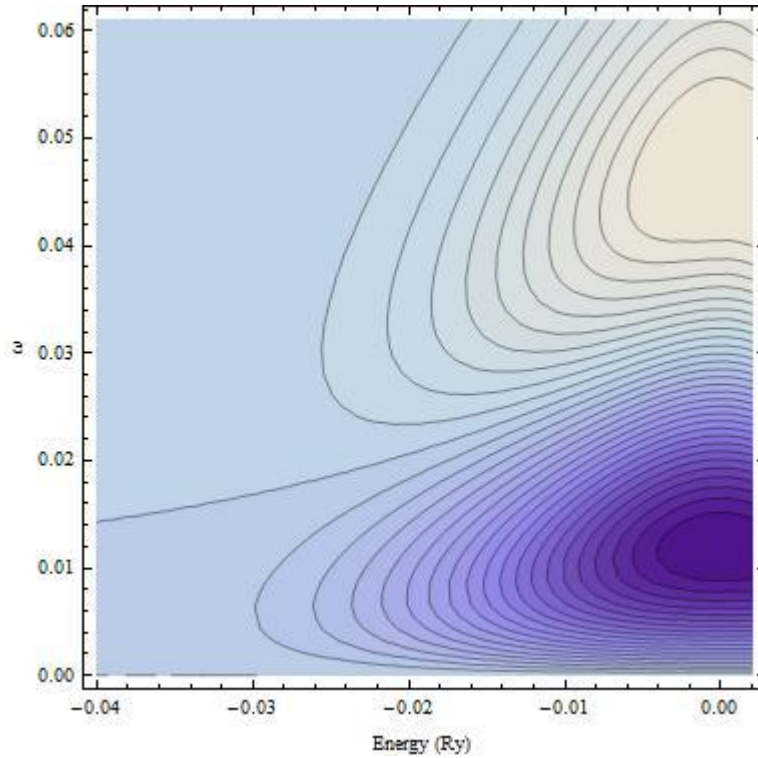


Figure 4.5 Contour plot for $C = 5$, $L = 100$, where the y-axis is the frequency $\omega(E)$ and the x-axis is the energy E in Rydberg units.

For $C = 5$, $L = 100$ we get

$$\omega(E) = 0.036 + (0.451)E + (-6.210)E^2 + (-190.76)E^3 \quad (4.8)$$

and for $C = 5$, $L = 50$ we get

$$\omega(E) = 0.061 + (0.391)E + (-4.457)E^2 + (-60.01)E^3 \quad (4.9)$$

as shown in figure 4.6.

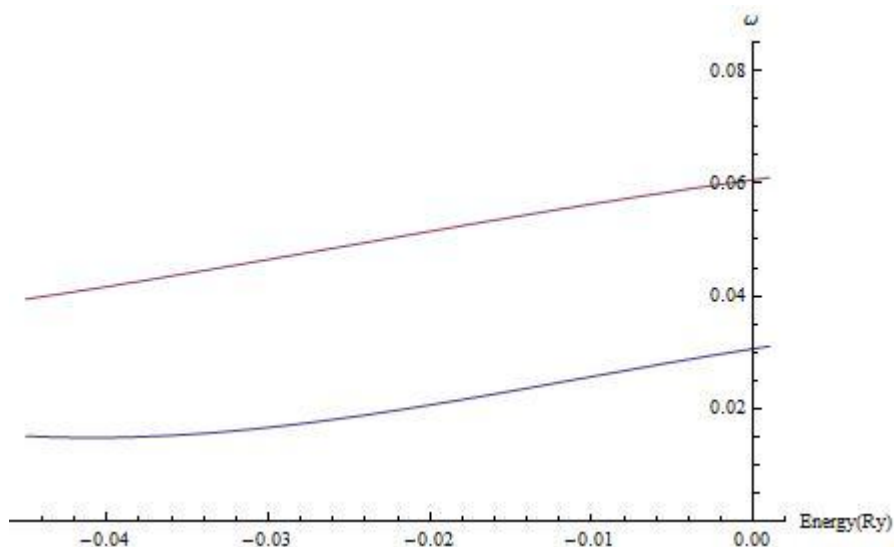


Figure 4.6 Graph of $\omega(E)$ from minimal total energy. The blue line (below) is $\omega(E)$ for $C = 5$, $L = 100$ (4.8) and the red line (above) is $\omega(E)$ for $C = 5$, $L = 50$ (4.9) in Rydberg units.

We can see that the $\omega(E)$ is lower when L is large. If the correlation length is large, the $\omega(E)$ will reach 0 for free particle case (no oscillation).

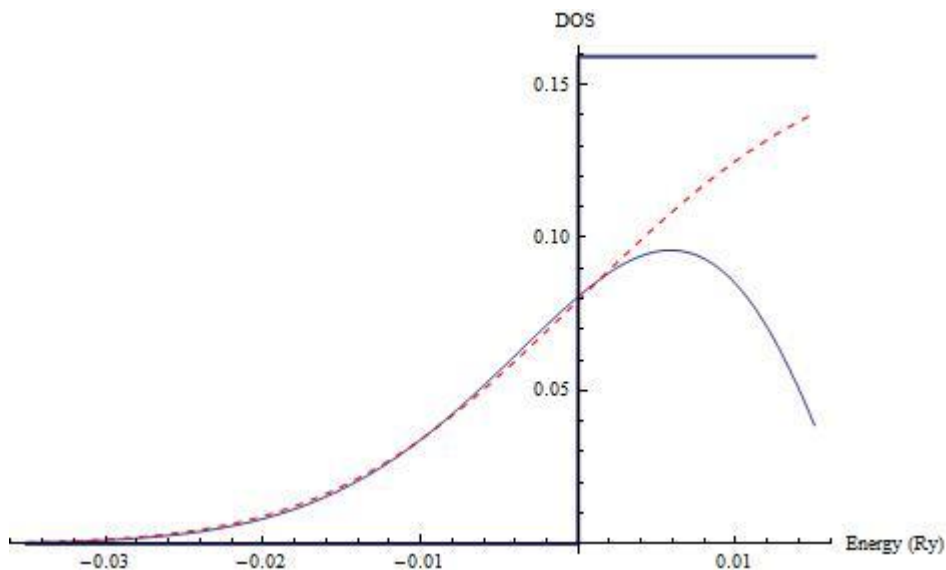


Figure 4.7 The DOS (4.2) from minimal total energy (blue line), the DOS (4.1) of semiclassical approximation (red dashed line) and the free particle DOS (1.19) (thick line), for $C = 5$, $L = 100$ in Rydberg units.

Again we can see that the whole results are not connected (Figure 4.7). So, we need to find the variational way to get the ω to make the positive and negative DOS joint together.

4.3 Density of states from touching slope method.

It is natural to obtain the smooth DOS. Now, we impose the conditions that

1. The DOS of tail must touch with the DOS from semiclassical.
2. The touching point must have the same slope.

For $C = 5$, $L = 100$, we get $\omega = 0.256$. The frequency is quite large when we compare with the others.

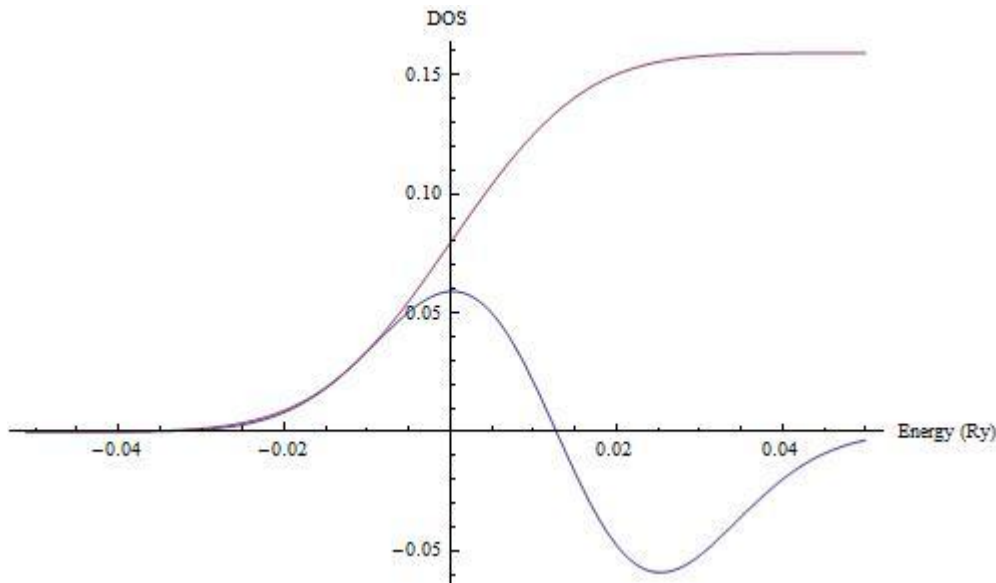


Figure 4.8 For $C = 5$, $L = 100$, the DOS from touching slope method (4.2) (blue line) and the DOS from semiclassical approximation (4.1) (red line) in Rydberg units.

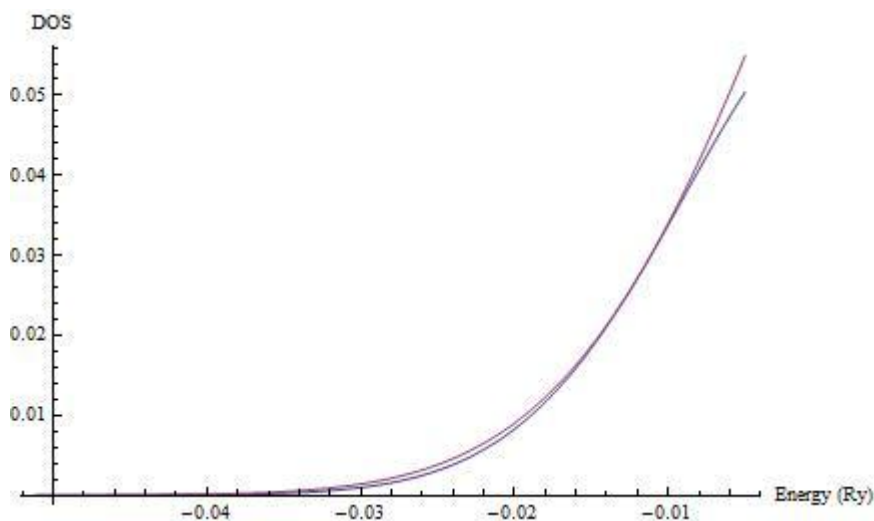


Figure 4.9 The tail region for density of states in Figure 4.8.

The DOS is very close to semiclassical and in the lower touching point, this method gives lower value for the DOS.

4.4 Density of states from tuning frequency method.

We try to find the frequency that makes the highest value of negative DOS touch the free particle DOS. This method has some advantages.

1. The experimental results show that the DOS and its slope are continuous.
2. The semiclassical DOS have anti-symmetrical shape along y-axis but real DOS do not have the anti-symmetrical shape because of the effect of impurities.

The condition we imposed fit with the experiments and we will see later that the frequency (ω) from this method are not much different from other methods in some energy range. At high and low energy limit, the result reaches the semiclassical approximation.

In this model, we simply assume the frequency (ω) does not change much in the energy range that we have considered. If we choose $C = 5$, $L = 100$ the frequency we get is $\omega = 0.0420845$ and the DOS we obtain by tuning frequency is the blue line and the semiclassical DOS is the red line (Fig.4.10)

The negative value is very close to semiclassical DOS. The trap state is continued from $-\infty$ and stops very sharply at $E = 0.008461$ (orange shade in Figure 4.11), with the free particle states above (blue shade in Figure 4.11), while the semiclassical DOS do not have clear conjunction between trap and free particle states.

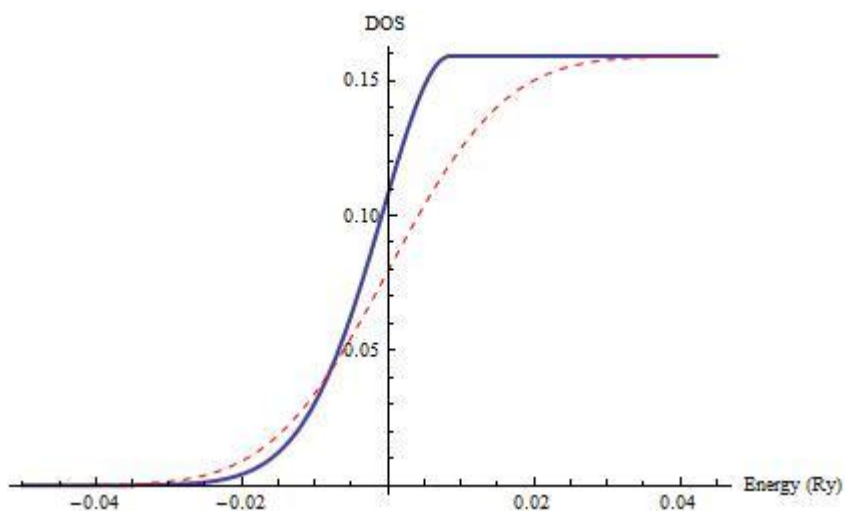


Fig.4.10 Show the semiclassical DOS (4.1) (red dashed line) , the DOS from the tuning frequency method (thick line) in Rydberg units.

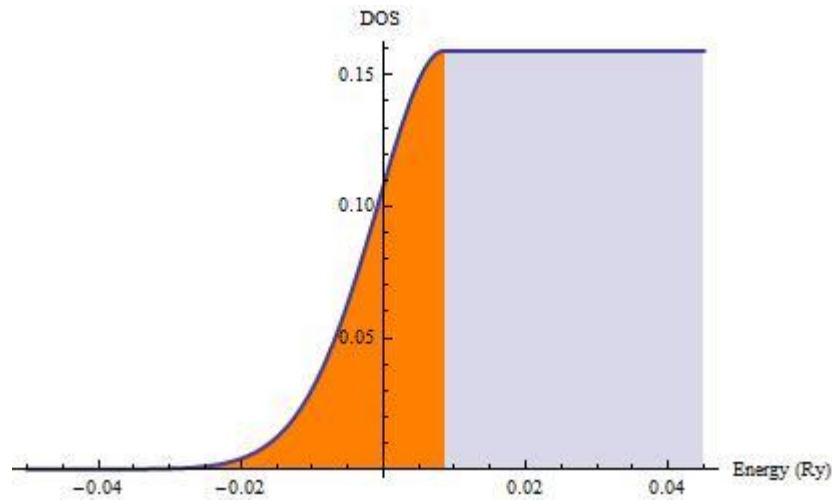


Figure 4.11 The trap states (4.2) (orange shade) joined with the free states (blue shade).

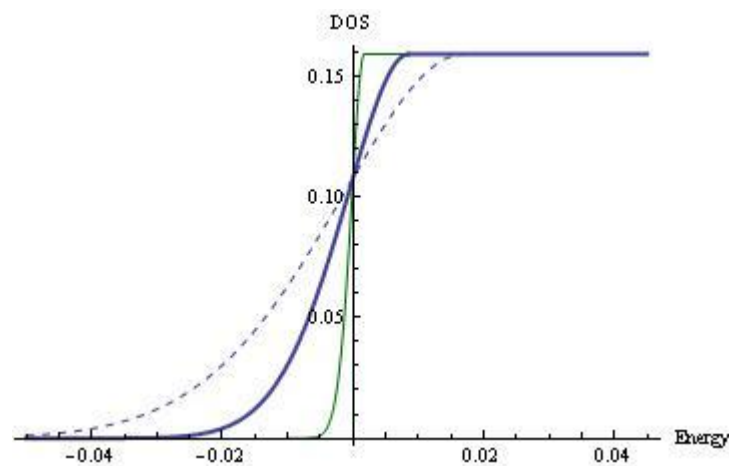


Figure 4.12 The DOS from tuning frequency method for various correlation length (L), $L = 50$ (dashed line), $L = 100$ (thick line), $L = 500$ (thin green line) and x-axis is energy in Rydberg unit.

In the case of $C = 5$ and vary L (Fig 4.12), it means that we change the concentration of the impurities. The slope decreases when the correlation length decreases. So, when $L \rightarrow \infty$ the DOS is close to the step function.

The very important consequence from unsymmetrical DOS is the shifting of Fermi level. Suppose our two-dimensional system has N number of particles that are fixed and the temperature is not so high. We simply have found the total number of electrons [28] by

$$N = \int D(E')dE' \quad (4.10)$$

The DOS of free electrons is step function. The potential of the impurities will present additional bound states for some negative energy range and reduce some free states in positive energy range. The number of particles should be conserved, so the particles emerging in negative energy range will be equal to the particles disappear from positive energy range.

We can now conclude that that Fermi-Level will be shifted [29].

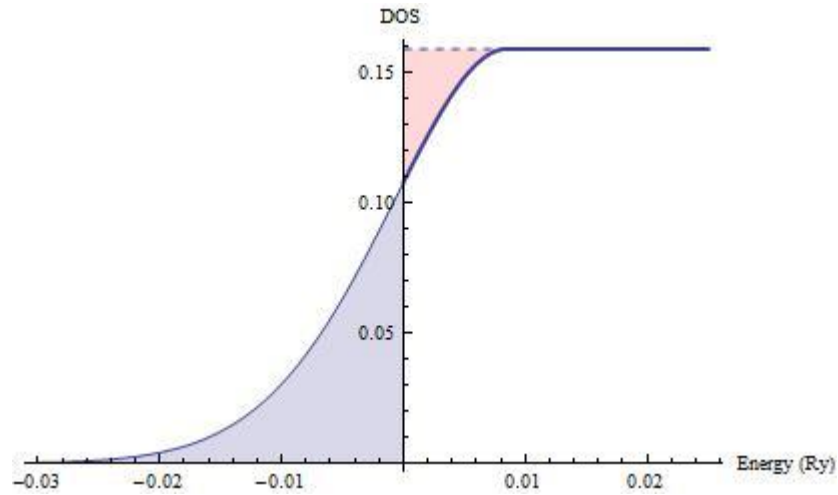


Figure 4.13 The number of particles increased in bound states (blue area), the number of particles decreased in bound states from the tuning frequency method (pink area).

For $C = 5$, $L = 100$ the blue region has an area 0.00809038 while the upper pink region has an area 0.000161272. So, the Fermi-level will decrease 0.00407004 as shown in figure 4.13.

The result is different from semiclassical model because the semi-classical model has symmetric DOS.

By this method, if we fix $L = 100$ (concentration of doping) and then vary C . It means that we change the strength of the interaction by changing the doping substrate. The results are shown in table 4.1.

C (strength of the interaction)	ΔN
0.001	0.00000663
0.01	0.0000262
0.1	0.0000890
1	0.000288
5	0.000648
10	0.000917
100	0.00206
500	0.00651

Table 4.1 The numerical relation between C (strength of the interaction) and ΔN . $\Delta N \equiv$ number of particles increasing in negative energy region - number of particles decreasing in positive energy region.

From the result we can see that when $C \rightarrow 0$, DOS is coming close to semiclassical limit because they become more symmetric and closer to the step function too. But when we are increasing C , the number of particles in negative energy will be increased, so the Fermi-level will be more shifted down.

If we assume that the number of particles in our system is very large. The shifting can be shown as

$$\Delta E_f = \frac{\Delta N}{\left(\frac{m}{\pi \hbar^2}\right)}. \quad (4.11)$$

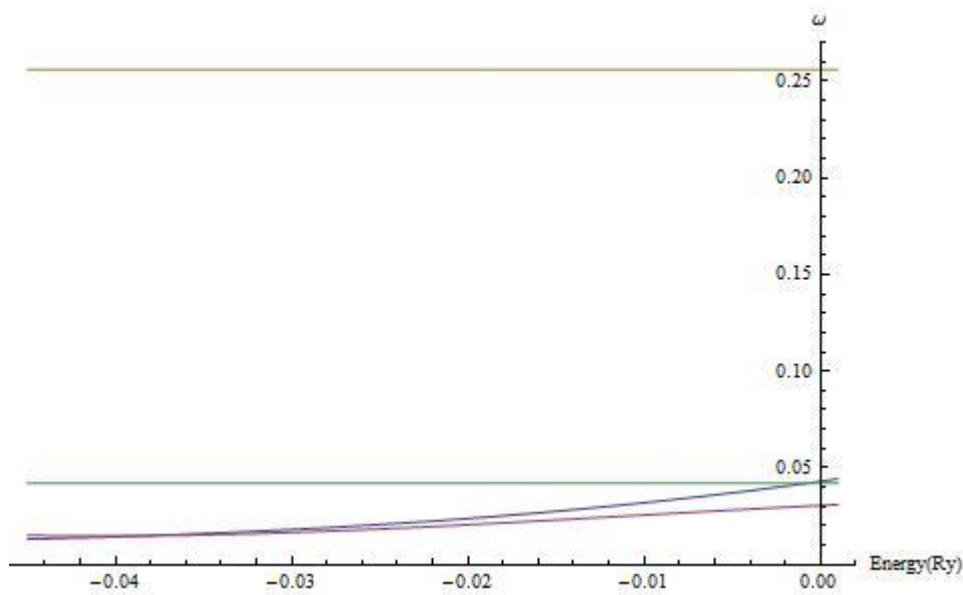


Figure 4.14 For $C = 5$, $L = 100$, the blue line is $\omega(E)$ from maximized DOS, the red line is $\omega(E)$ from minimal total energy, the yellow line is $\omega(E)$ from touching slope method and the green line is $\omega(E)$ from tuning frequency method in Rydberg units.

All frequency is shown in figure 4.14 and we can see that the touching slope method has very different frequency but the frequency from other methods is quite similar. The DOS from touching slope method is similar with the semiclassical method, so this method cannot describe the tail states and the frequency from this method is not the frequency of the system.

The DOS from tuning frequency method is smooth, and do not have the discontinuous problem. The shifting of Fermi-level can be predicted from the tuning frequency method and the frequency from this method is constant but it does not differ much from other two, so it can represent the frequency of the real system. We can analyze the system more easily because the frequency from this method is constant and the DOS of tail states (4.2) and free states (1.19) are joined.

CHAPTER V

Conclusions

Path integral method provides solutions for two dimensional semiconductor systems. In our research, we use the new variational method to join the band tail states with the semiclassical DOS smoothly. Our method has removed the discontinuous problem for the DOS. We have shown and compared the frequencies from the several variational methods and observed that the frequency from maximized DOS method, minimum the total energy method and tuning frequency method are not differing much and all frequency values become closer together when energy approaches zero. The different frequency leads to the different DOS. However, if we consider only the band tail region, they are quite similar.

We also calculated the number of particles increasing in the band tail states and the number of particle disappearing in the free particle states. This effect can be explained by the electrons in conduction band interacting with the impurities being possible to form bound states with the impurities. Since the number of electrons in the system is constant, electrons in free particle states can move to fill bound states, so the number of electrons in free particle states will be decreased and the number of electrons in bound particle states will be increased. Our variational method can estimate the Fermi-level shift when the effect of impurities is present. Higher strength of Gaussian interaction contributes more particles bound in the tails region, so the Fermi-level will be more shifted down.

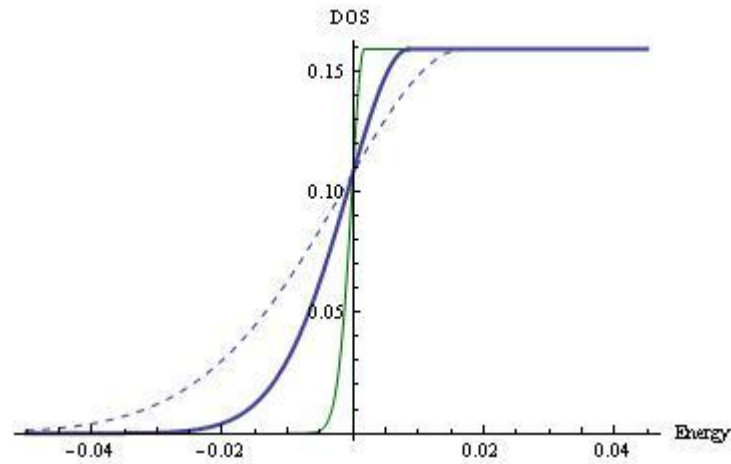


Figure 5.1 The DOS from tuning frequency method for various correlation length (L), $L = 50$ (dashed line), $L = 100$ (thick line), $L = 500$ (thin green line) and x-axis is energy in Rydberg unit.

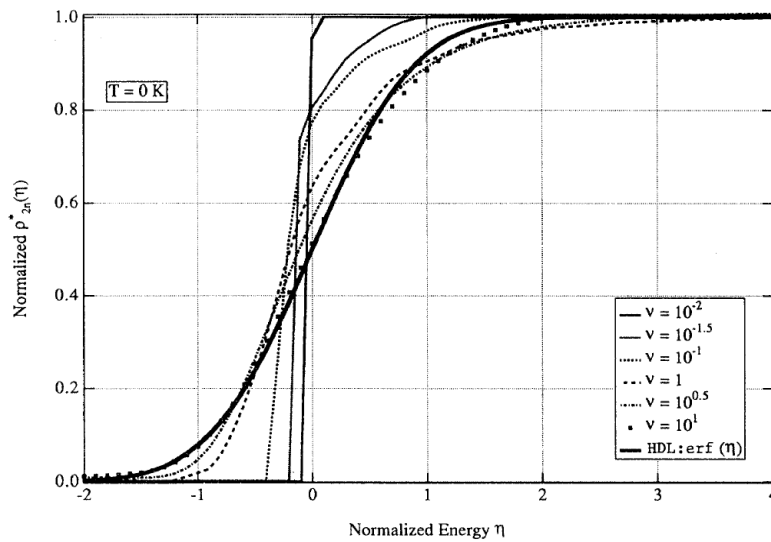


Figure 5.2 The DOS from generalized semiclassical model for various impurities concentration [30].

Our method makes two DOS joined together. The impurities concentration is a very important parameter to our method. When the system has low concentration, the DOS reach the step function and the joining point between negative DOS and free DOS gets lower. If the impurities are doped with more concentration, we observe more negative DOS in the positive energy region (figure 5.1). The important features from our theory is after we calculated the

frequency, we can analyze the DOS of the two dimensional semiconductors easily by using the negative DOS for negative energy region to the joining point and then switch to the free DOS to describe the positive energy states. We can compare our results with the generalized semiclassical model that was able to explain the absorption data of doped GaAs quantum wells [31].

The tuning frequency method gives the same DOS values for various correlation lengths when energy reaches zero, while the generalized semiclassical model [30] do not. If energy reaches zero, the generalized semiclassical model gives high DOS when impurities concentration is low. The result of the generalized semiclassical model is more realistic because when the impurities are doped, bound states are present. Hence, DOS at zero energy will be decreased. However, the whole result do not change much and the important thing we have discovered from the tuning frequency method is this method give analytic form of DOS that we can move further to find other physical variables (relaxation time, current density of electrons and specific heat capacity) more conveniently.

References

- [1] Hang, D. R., et al. Effective mass of two-dimensional electron gas in an Al_{0.2}Ga_{0.8}N/GaN heterojunction. Applied Physics Letter 79 (2001): 66-68
- [2] Gold, A. Electronic transport properties of a two-dimensional electron gas in a silicon quantum-well structure at low temperature. Physical Review B 35 (1987): 723-733
- [3] Salis, M. Thomas-Fermi Screening in Graphene, [arXiv:cond-mat/0701108v2](https://arxiv.org/abs/cond-mat/0701108v2) (2007)
- [4] Katsnelson, M. I. Scattering of charge carriers by point defects in bilayer graphene. Physical Review B 76 (2007): 73411
- [5] Streetman, B. G. and Banerjee S. Solid State Electronic Devices. New Jersey: Prentice-Hall, (2000)
- [6] Middleton, W. and Van Valkenburg, M. E. Reference Data for Engineers: Radio, Electronics, Computers and Communications. Boston: Newnes, (2002)
- [7] Kittel, C. Introduction to Solid State Physics. New York: John Wiley & Sons, (2004)
- [8] Ashcroft, N. W., and Mermin, D. N. Solid State Physics., Brooks/Cole, (1976)
- [9] Wofff, P. A. Theory of the band structure of very degenerate semiconductors. Physical Review 126 (1962): 405-412
- [10] Kane, E. O. Thomas-Fermi approach to impure semiconductor band structure. Physical Review 131 (1963): 79-88
- [11] Halperin, B. I., and Lax, M. Impurity-band tails in the high-density limit. I. Minimum counting methods. Physical Review 148 (1966): 722-740

- [12] Saitoh, M., and Edwards, S. F. A note on the density of states of a disordered system with Gaussian random potentials. Journal of Physics C: Solid State Physics 7 (1974): 3937-40
- [13] Lloyd, P., and Best, P. R. A variational approach to disordered systems. Journal of Physics C: Solid State Physics 8 (1974): 3752-3766
- [14] Sritrakool, W., Sa-yakanit, V., and Glyde, H. R. Band tails in disordered systems. Physical Review B 33 (1986): 1199-1202
- [15] Thongnum, A., Pinsook, U., and Sa-yakanit, V. Interface roughness effect on density of states and mobility of narrow Si/Si(1-x)Ge(x) quantum wells: path-integral approach. Journal of Physics D: Applied Physics 42 (2009): 195101
- [16] Mukhanov, V. F., and Winitzki, S. Intruduction to Quantum Effect in Gravity. New York: Cambridge University Press, (2007)
- [17] Kaku, M. Quantum Field Theory: A Modern Introduction. New York: Oxford University Press, (1993)
- [18] Sakurai, J. J. Modern Quantum Mechanics. Addison-Wesley, (1994)
- [19] Feynman, R. P., and Hibbs, A. R. Quantum Mechanics and Path Integrals. McGraw-Hill, 1965
- [20] Sa-yakanit, V., and Glyde, H. R. Impurity-band density of states in heavily doped semiconductors: A variational calculation. Physical Review B 22 (1980): 6222-6232
- [21] Van Mieghem, P. Theory of band tails in heavily doped semiconductors. Reviews of Modern Physics 64 (1992): 755-793
- [22] Kubo, R. Generalized cumulant expansion method. Journal of the Physical Society of Japan 17 (1962)

- [23] Dittrich, W., and Reuter, M. Classical and Quantum Dynamics: From Classical Paths to Path Integrals. New York: Springer, (2001)
- [24] Samathiyakanit, V. Path-integral theory of a model disordered system. Journal of Physics C: Solid State Physics 7 (1974): 2849
- [25] Schulman, L. S., and Dewitt-Morette, C. Technique and applications of path integration. New York: Dover Publications, 1981
- [26] Quang, D. N., and Tung, N. H. Deep tail in the density of states of a disordered two-dimensional electron gas. Physica Status Solidi (b) 209 (1998): 375-387
- [27] Walter, A. H. Solid State Theory. Dover Publications, 1980
- [28] Sa-yakanit, V. Electron density of states in a Gaussian random potential: Path-integral approach. Physical Review B 19 (1979): 2266-2275
- [29] Nam-Young, L., Kyu-Jang, L., Chul, L., Jae-Eun, Kim, and Hae Yong Park. Determination of conduction band tail and Fermi energy of heavily Si-doped GaAs by room- temperature photoluminescence. Journal of Applied Physics 78 (1995): 3367-3370
- [30] Van Mieghem, P., Borghs, G., and Mertens, R. Generalized semiclassical model for the density of states in heavily doped semiconductors. Physical Review B 44 (1991): 12822-12829
- [31] Knox, W. H., Chemla, D. S., Livescu, G., Cunningham, J. E., and Henry, J. E. Femtosecond carrier thermalization in dense Fermi seas. Physical Review Letters 61 (1988): 1290-1293

APPENDICES

APPENDIX A

Baker–Campbell–Hausdorff formula

We will prove Baker–Campbell–Hausdorff formula

$$\exp(G\lambda)A\exp(-G\lambda) = A + \lambda[G, A] + \frac{\lambda^2}{2!}[G, [G, A] + \dots O(\lambda^3)], \quad (\text{A1})$$

where G and A are any operator and λ is any scalar function,

$$\begin{aligned} \exp(G\lambda)A\exp(-G\lambda) &= \left(1 + G\lambda + \frac{\lambda^2}{2!}G^2 + \dots\right) A \left(1 - G\lambda + \frac{\lambda^2}{2!}G^2 + \dots\right) \\ &= \left(1 + G\lambda + \frac{\lambda^2}{2!}G^2 + \dots\right) \left(A - AG\lambda + \frac{\lambda^2}{2!}AG^2 + \dots\right). \end{aligned} \quad (\text{A2})$$

Now, we expand and try to group same order of λ together

$$\begin{aligned} \exp(G\lambda)A\exp(-G\lambda) &= A + \lambda[G, A] + \frac{\lambda^2}{2!}(AG^2 - GAG - GAG + G^2A) + \dots O(\lambda^3) \\ &= A + \lambda[G, A] + \frac{\lambda^2}{2!}((AG - GA)G - G(AG - GA)) + \dots O(\lambda^3) \\ &= A + \lambda[G, A] + \frac{\lambda^2}{2!}([A, G]G - G[A, G]) + \dots O(\lambda^3) \\ &= A + \lambda[G, A] + \frac{\lambda^2}{2!}(G[G, A] - [G, A]G) + \dots O(\lambda^3) \\ &= A + \lambda[G, A] + \frac{\lambda^2}{2!}([G, GA] - [G, AG]) + \dots O(\lambda^3) \\ &= A + \lambda[G, A] + \frac{\lambda^2}{2!}([G, GA - AG]) + \dots O(\lambda^3) \\ &= A + \lambda[G, A] + \frac{\lambda^2}{2!}([G, [G, A]]) + \dots O(\lambda^3). \end{aligned} \quad (\text{A3})$$

The Eq.(A3) is called the Baker–Campbell–Hausdorff formula, we will use it to prove this formula

$$e^{A+B} \approx e^A e^B e^{-\frac{1}{2}[B, A]}. \quad (\text{A4})$$

Since G is an arbitrary operator, we can choose to define G in the form

$$G(\lambda) = e^{\lambda A} e^{\lambda B}, \quad (\text{A5})$$

where λ is any scalar function. Then we take the derivative on G

$$\begin{aligned}
\frac{dG}{d\lambda} &= Ae^{\lambda A}e^{\lambda B} + e^{\lambda A}Be^{\lambda B} \\
&= AG + e^{\lambda A}Be^{-\lambda A}e^{\lambda A}e^{\lambda B} \\
&= (A + e^{\lambda A}Be^{-\lambda A})G.
\end{aligned} \tag{A6}$$

By using Baker–Campbell–Hausdorff formula with the second term in the bracket, we obtain

$$\frac{dG}{d\lambda} = \left(A + B + \lambda[A, B] + \frac{\lambda^2}{2!}[A, [A, B]] + O(\lambda^3) \right) G. \tag{A7}$$

Then we integrate over G and λ ,

$$\begin{aligned}
\ln G &= \lambda A + \lambda B + \frac{\lambda^2}{2!}[A, B] + \frac{\lambda^3}{3!}[A, [A, B]] + O(\lambda^4) \\
G(\lambda) &= \exp\left(\lambda A + \lambda B + \frac{\lambda^2}{2!}[A, B] + \frac{\lambda^3}{3!}[A, [A, B]] + O(\lambda^4) \right).
\end{aligned} \tag{A8}$$

So we obtain

$$e^{\lambda A}e^{\lambda B} = \exp\left(\lambda A + \lambda B + \frac{\lambda^2}{2!}[A, B] + \frac{\lambda^3}{3!}[A, [A, B]] + O(\lambda^4) \right). \tag{A9}$$

To get the final result, we simply set limit $\lambda \rightarrow 1$

$$e^Ae^B = \exp\left(A + B + \frac{1}{2!}[A, B] + \dots \right). \tag{A10}$$

APPENDIX B

Functional calculus

In the random system, we have to deal with many averaged quantities. It is necessary to know the functional calculus.

$$K(q_f, q_0; t_f, t_0) = \int_{q_0}^{q_f} \mathbf{D}q \exp\left(\int_{t_0}^{t_f} \frac{i}{\hbar} dt L(q, \dot{q})\right) \quad (\text{B1})$$

The propagator is the functional integral because this integral has performed over all possible function $q(t)$. The result we get, $K(q_f, q_0; t_f, t_0)$ is the scalar quantity. This is mapping between function $q(t)$ to the number. It is clearly different from concept of function that maps between number to number. When we map function $q(t)$ to a number, we use the symbol $Q[q(t)]$. Note that $Q[q(t)]$ is the number for some form of $q(t)$.

Now, we define the functional derivative by analogy with ordinary derivative as

$$\frac{\delta Q[q(t)]}{\delta q(\tau)} = \lim_{\varepsilon \rightarrow 0} \frac{Q[q(t) + \varepsilon \delta(x-y)] - Q[q(t)]}{\varepsilon} \quad (\text{B2})$$

Then we introduce the useful relations

$$1. \text{ if } Q[q] = \int d\tau (q(\tau))^n \text{ then } \frac{\delta Q[q]}{\delta q(\tau)} = n(q(\tau))^{n-1}, \quad (\text{B3})$$

$$2. \text{ if } Q[q] = \int d\tau \left(\frac{dq(\tau)}{d\tau}\right)^n \text{ then } \frac{\delta Q[q]}{\delta q(\tau)} = -n \frac{d}{dt} \left(\frac{dq}{dt}\right)^{n-1} \Bigg|_{\tau}, \quad (\text{B4})$$

$$3. \text{ if } Q_y[q] = \int d\tau K(y, \tau) q(\tau) \text{ then } \frac{\delta Q_y[q]}{\delta q(\tau)} = K(y, \tau), \quad (\text{B5})$$

$$4. \text{ if } Q[q] = \exp\left(\int d\tau q(\tau) f(\tau)\right) \text{ then } \frac{\delta Q[q]}{\delta q(\tau)} = f(\tau) \exp\left(\int d\tau q(\tau) f(\tau)\right) \quad (\text{B6})$$

$Q_y[q]$ means this functional also depends on y coordinate. All relations above can be derived from the definition of functional derivative we have recently introduced.

APPENDIX C

The classical action of non-local force harmonic oscillator

We will find the classical action of a non-local force harmonic oscillator. There is a slight difference at the beginning point because we do not know the exact position of the oscillator. Therefore, the potential form (that depends on the position) must be changed. The form of the non-local simple harmonic potential is

$$V = \frac{m}{2(t_2 - t_1)} \omega^2 \int_{t_1}^{t_2} d\tau [x(s) - x(\tau)]^2. \quad (\text{C.1})$$

We take the average of the simple harmonic with time interval $(t_2 - t_1)$. But for convenience sake in calculation, we set $t_1 = 0$ and $t_2 = t' = \text{constant}$. The Lagrangian of our non-local potential is

$$L(x, \dot{x}) = \frac{m}{2} \dot{x}^2 - \frac{m}{2(t')} \omega^2 \int_0^{t'} d\tau [x(t) - x(\tau)]^2 + F(t)x. \quad (\text{C.2})$$

Now, take the derivative on x and \dot{x} to obtain the equation of motion

$$\frac{\partial L}{\partial x} = -\frac{m}{(t')} \omega^2 \int_0^{t'} d\tau [x(t) - x(\tau)] + F(t), \quad (\text{C.3})$$

$$\frac{\partial L}{\partial \dot{x}} = m\dot{x}, \quad (\text{C.4})$$

$$m\ddot{x} = -\frac{m}{t'} \omega^2 \int_0^{t'} d\tau [x(t) - x(\tau)] + F(t). \quad (\text{C.5})$$

We will perform the first integral and rearrange this equation

$$m\ddot{x} + m\omega^2 x(t) = \frac{m\omega^2}{t'} \int_0^{t'} d\tau x(\tau) + F(t). \quad (\text{C.6})$$

We see the extra term $\frac{m\omega^2}{t'} \int_0^{t'} d\tau x(\tau)$ emerging from our system. Unfortunately, we cannot simply add the extra term in our recent solution, because the answer of this differential equation is

$$x(t) = X_1 \cos[\omega(t)] + A \sin[\omega(t)] + \frac{1}{m\omega} \int_0^t d\tau \sin[\omega(t-\tau)] \left(\frac{m\omega^2}{t'} \int_0^{t'} dsx(s) + F(\tau) \right), \quad (\text{C.7})$$

where

$$A = (X_2 - X_1 \cos(\omega t')) \frac{1}{\sin(\omega t')} - \frac{1}{m\omega \sin(\omega t')} \int_0^{t'} d\tau \sin[\omega(t'-\tau)] \left(\frac{m\omega^2}{t'} \int_0^{t'} dsx(s) + F(\tau) \right). \quad (\text{C.8})$$

The solution can be checked directly by substituting it in (C.6). This is not finished because the solution is not all explicit. We can see the $x(s)$ in the right hand side remaining in the integral so this solution is an integral equation. One way to solve this integral equation is “the direct computational method”.

Our problem can be written in the form

$$u(t) = f(t) + \lambda g(t) \int_a^b ds h(s) u(y), \quad (\text{C.9})$$

$$x(t) = \left(X_1 \cos[\omega(t)] + A \sin[\omega(t)] + \frac{1}{m\omega} \int_0^t d\tau \sin[\omega(t-\tau)] F(\tau) \right) + \frac{\omega}{t'} \left(\int_0^t d\tau \sin[\omega(t-\tau)] \right) \int_0^{t'} dsx(s). \quad (\text{C.10})$$

There are many methods to get the classical action. V. Samathiyakanit derived the equivalent result in 2 ways and get the same results [24]

$$S = \frac{m\omega}{4} \cot\left(\frac{1}{2}\omega t\right) |X_2 - X_1|^2 + \frac{m\omega}{2\sin(\omega t)} \left\{ \frac{2X_2}{m\omega} \int_0^t d\tau F(\tau) \left(\sin(\omega\tau) - 2\sin\left(\frac{1}{2}\omega\tau\right) \sin\left[\frac{1}{2}\omega(t-\tau)\right] \sin\left(\frac{1}{2}\omega\tau\right) \right) \right. \\ \left. + \frac{2X_1}{m\omega} \int_0^t ds F(s) \left(\sin[\omega(t-s)] - 2\sin\left(\frac{1}{2}\omega t\right) \sin[\omega(t-s)] \sin\left(\frac{1}{2}\omega s\right) \right) \right. \\ \left. - \frac{2}{(m\omega)^2} \int_0^t dt \int_0^{\tau} ds F(s) F(t) \sin[\omega(t-\tau)] \sin[\omega(s)] \right\}$$

$$-4 \sin\left[\frac{1}{2}\omega(t-\tau)\right] \sin\left[\frac{1}{2}\omega(\tau)\right] \sin\left[\frac{1}{2}\omega(t-s)\right] \sin\left(\frac{1}{2}\omega s\right) \Big\}. \quad (\text{C.11})$$

(C.11) is the classical action of force in harmonic oscillator of the non-local system. If we are interested in the case of no driven force, we simply set $F = 0$ and get

$$S_0 = \frac{m\omega}{4} \cot\left(\frac{1}{2}\omega t\right) |X_2 - X_1|^2, \quad (\text{C.12})$$

the classical action of free harmonic oscillator of the non-local system.

APPENDIX D

The distribution function of random potential

We assume the impurities are doped randomly in the system. The probability of finding one impurity will be constant in all positions. If our system is large, the probability to see the impurity will be small. We can simply write this statement as

$$p(r_i, V) \propto \frac{1}{V_0} , \quad (\text{D1})$$

where $p(r_i)$ is the probability to find the potential V at point r_i , and V_0 is the volume of the system. So, we will obtain the total probability by multiplying all together

$$P(r, V) = \int \frac{1}{V_0} dr_1 \int \frac{1}{V_0} dr_2 \dots \int \frac{1}{V_0} dr_N \delta(V(r) - V(r - \{r_i\})), \quad (\text{D2})$$

where $\{r_i\}$ is the average impurity position, N is number of the impurity. Our total potential can be written in the form $V(r) = \sum_{i=1}^N v(r - r_i)$. We rewrite Eq.D2 by using the identity

$$\delta(y - a) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(y-a)x} dx ,$$

then we get the total probability as

$$P(r, V) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{iVx} \int_{V_0} \left[dR \frac{1}{V_0} e^{-iv(r-R)x} \right]^N dx . \quad (\text{D3})$$

VITAE

Mister Ardwarong Jantamas was born on August 5, 1984 in Ubonratchathani, Thailand. He has been a student in the Development and Promotion for Science and Technology Talents Project (DPST). He had received his Bachelor Degree of Science Program in Physics from the Department of Physics, Faculty of Science, Mahidol University in 2006, and continued his Master's study in 2007. He has also participated one conference, as follows:

- [1] **Jantamas A.**, Pinsook U. and Sa-yakanit V. Electronic density of states of random Thomas Fermi potential in 2 dimensions, *17th National Graduate Research Conference, Buriram, Thailand (2010)* (Poster)