CHAPTER III

PATH INTEGRAL METHOD

3.1 Introduction

As discussed in Chapter II, the theory of Halperin and Lax[5,9] is successful for computing the density of states for the one - dimensional white noise model, but for the application purposes it has two limitations[11].It first of all requires numerical solution. Secondly it can not be extended to higher energy E. For these reasons, Sa-yakanit developed a new approach[10] based on the Feynman formulation of quantum mechanics.[12] His method gives an analytic expression of $\rho(E)$ which is valid at all energies E for disordered systems having a screened coulomb potential. For the one - dimensional white noise potential, the density of states can be easily calculated, and is found to be in good agreement with the exact result. Before going to the discussion on our work in the next chapter, we devote this chapter to review Sa-yakanit's work which we call " the leading term approximation in first cumulant."

3.2 Density of States

It is convenient to consider the density of states in the form which is defined by (2.2.4)

$$\rho(E) = \frac{1}{\Omega} < \sum_{i=1} \delta(E - E_i)>, \qquad 2.2.4$$

where E_i is the energy of the i th eigenstate of a Hamiltonian, Ω is a container of N scatterers in d dimension, and where the angular

bracket < > indicates an average over an ensemble of the scatterer positions.

To apply the path integral method to (2.2.4), one converts the right-hand side of (2.2.4) into an integral form to get[10]

$$\rho(E) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt\, e^{iEt/\hbar}\, \mathrm{Tr}\, G(\vec{X}_2, \vec{X}_1; t), \qquad 3.2.1$$

where the operation Tr denotes the trace of G, the function G is a retarded propagator describing the propagation of an electron from point $\vec{X}_1$ to $\vec{X}_2$, and where $\vec{X}_1$ and $\vec{X}_2$ are vector positions of the electron in d dimensions.

Because the propagator G is an average propagator of an average system, the propagator G is invariant under translation of $\vec{X}$. This means that

$$G(\vec{X}_2, \vec{X}_1; t) \equiv G(\vec{X}_2 - \vec{X}_1, 0\,;\, t). \qquad 3.2.2$$

For finding the density of states, the end point $\vec{X}_2$ and the initial point $\vec{X}_1$ must be the same. It therefore follows that

$$\rho(E) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt\, e^{iEt/\hbar}\, G(0,0;t). \qquad 3.2.3$$

3.3 Gaussian Random Model

To evaluate the propagator G mentioned in the preceding section, we first consider a simple model which can be conveniently expressed in

terms of Feynman - like path integrals.[12,14,15] The model is that of an electron in a system of very dense, random, weak scatterers. If $\bar{N}$ is the density of the scatterers, and $v(\vec{X})$ is the scattering potential, then the model is obtained by taking the limits[13]

$$\lim_{GRM} = \lim_{(\bar{N} \to \infty,\ v \to 0,\ \bar{N}v^2 \to \text{finite})} . \qquad 3.3.1$$

To begin the calculation in the limit of (3.3.1), we first consider a propagator $\tilde{G}(\vec{X}_2, \vec{X}_1; t, [\vec{R}_i])$ for an electron in the presence of N scatterers at the fixed positions $\{\vec{R}_i \mid i = 1,\ldots, N\}$. It is obvious that this propagator must depend explicitly on the positions of the scatterers. Since the scatterers are randomly distributed, such properties of the system as the density of states are obtained from the average propagator $G(\vec{X}_2, \vec{X}_1; t)$, the average of $\tilde{G}$ over the random scatterer positions.

For the model of N scatterers, the Hamiltonian for the electron is

$$H([\vec{R}_i]) = -\frac{\hbar^2}{2m}\nabla^2 + \sum_{i=1}^{N} v(\vec{X}(\tau) - \vec{R}_i), \qquad 3.3.2$$

where m is the electron mass, and v is the scattering potential at the position $\vec{X}$. The position $\vec{R}_i$ of the scatterers are taken to be random. The probability for the scattering centers to be at $\vec{R}_i$ is, therefore

$$P([\vec{R}_i]) = \frac{1}{\Omega^N} \qquad 3.3.3$$

where Ω is the volume of the system .

The propagator of such a system satisfies

$$[i\hbar\frac{\partial}{\partial t} - H([\vec{R}_i])]\tilde{G}(\vec{X}_2, \vec{X}_1; t, [\vec{R}_i]) = i\hbar\delta(\vec{X}_2 - \vec{X}_1)\delta(t). \qquad 3.3.4$$

In the path integral representation, the propagator is expressed as

$$\tilde{G}(\vec{X}_2, \vec{X}_1; t, [\vec{R}_i]) = \int \mathcal{D}[\vec{X}(\tau)] \exp\left\{\frac{i}{\hbar}\int_0^t d\tau\left[\frac{m}{2}\dot{X}^2(\tau) - \sum_{i=1}^{N} v(\vec{X}(\tau) - \vec{R}_i)\right]\right\}, \qquad 3.3.5$$

where $\mathcal{D}[\vec{X}(\tau)]$ denotes "the path integral" to be carried out with the boundary conditions $\vec{X}(0) = \vec{X}_1$ and $\vec{X}(t) = \vec{X}_2$. The average propagator is thus

$$G(\vec{X}_2, \vec{X}_1; t) = \langle\tilde{G}(\vec{X}_2, \vec{X}_1; t, [\vec{R}_i])\rangle$$

$$= \Omega^{-N}\int\cdots\int \prod_{i=1}^{N} d\vec{R}_i \tilde{G}(\vec{X}_2, \vec{X}_1; t, [\vec{R}_i]). \qquad 3.3.6$$

Since (3.3.6) implies that the average propagator G is the usual Green's function, G can be thought to describe the propagation of a particle, even though it does not correspond to a physical electron in a specific configuration. The function G can also be considered as a propagator describing the motion of a fictitious " average electron " in the average system.

As pointed out first by Edwards and Gulyaev[16], the average of

(3.3.6) can be explicitly obtained because the set of the positions $\{\vec{R}_i\}$ is random. Therefore the scattering potential $v(\vec{X}(\tau) - \vec{R}_i)$ are independent random variables,[17,18]

$$G(\vec{X}_2,\vec{X}_1; t) = \int \mathcal{D}[\vec{X}(\tau)] \exp\left\{ \frac{i}{\hbar} \cdot \frac{m}{2} \int_0^t d\, \dot{X}^2(\tau) + \bar{N} \int d\vec{R} \left[\exp\left(-\frac{i}{\hbar} \int_0^t d\tau v(\vec{X}(\tau) - \vec{R})\right) - 1\right]\right\},$$

3.3.7

where the density $\bar{N} = N/\Omega$. In the limit of (3.3.1), we can expand the exponential of v, and then keep only the linear and quadratic terms. The average potential

$$E_o = \bar{N} \int d\vec{R} v(\vec{X}(\tau) - \vec{R}), \qquad 3.3.8$$

becomes infinite in the limit (3.3.1). However, we are free to choose our energy origin as the average of energy for removing the infinite. Now we consider the quadratic term

$$-\frac{\bar{N}}{2\hbar^2} \int d\vec{R} \int_0^t \int_0^t d\tau d\sigma v(\vec{X}(\tau) - \vec{R}) v(\vec{X}(\sigma) - \vec{R}) = -\frac{\bar{N}}{2\hbar^2} \int_0^t \int_0^t d\tau d\sigma W[\vec{X}(\tau) - \vec{X}(\sigma)], \qquad 3.3.9$$

where the correlation function

$$W[\vec{X}(\tau) - \vec{X}(\sigma)] = \int d\vec{R}\, v(\vec{X}(\tau) - \vec{R})\, v\,(\vec{X}(\sigma) - \vec{R}). \qquad 3.3.10$$

In the limit of (3.3.1), Eq. (3.3.7) becomes

$$G(\vec{X}_2,\vec{X}_1;t) = \int \mathcal{D}[\vec{X}(\tau)]\exp\left\{\frac{i}{\hbar}\cdot\frac{m}{2}\int_0^t d\tau\dot{\vec{X}}^2(\tau) - \frac{i}{\hbar}E_o t - \frac{\bar{N}}{2\hbar^2}\int_0^t\int_0^t d\tau d\sigma W[\vec{X}(\tau)-\vec{X}(\sigma)]\right\}. \quad 3.3.11$$

We note that the correlation function (3.3.10) depends explicitly on the scattering potential employed, and (3.3.11) can be formally written in terms of an action S as

$$G(\vec{X}_2,\vec{X}_1;t) = \int \mathcal{D}[\vec{X}(\tau)]\exp\{\frac{i}{\hbar}S\}, \quad 3.3.12$$

where

$$S = \frac{m}{2}\int_0^t d\tau\dot{\vec{X}}^2(\tau) - E_o t + \frac{i}{2\hbar}\bar{N}\int_0^t\int_0^t d\tau d\sigma W[\vec{X}(\tau)-\vec{X}(\sigma)]. \quad 3.3.13$$

In order to find (3.3.12), we consider the Gaussian potential

$$v(\vec{X}(\tau)-\vec{R}) = u\eta(\pi\ell^2)^{-d/2}\exp\left\{-\frac{|\vec{X}(\tau)-\vec{R}|^2}{\ell^2}\right\}, \quad 3.3.14$$

where d denotes the dimension of the system, the constant $u\eta$ is the energy unit, and η is the strength of the scattering potential. We find that for the potential (3.3.14), Eq.(3.3.10) becomes

$$W[\vec{X}(\tau)-\vec{X}(\sigma)] = u^2\eta^2(\pi L^2)^{-d/2}\exp\left\{-\frac{|\vec{X}(\tau)-\vec{X}(\sigma)|^2}{L^2}\right\}, \quad 3.3.15$$

where L denotes the correlation length of the random system related to ℓ by

$$L^2 = 2\ell^2. \quad 3.3.16$$

In order to calculate W in the next section, we write

$$W(\vec{X}) = \int \frac{d^d\vec{k}}{(2\pi)^d} V(\vec{k}) \exp(i\vec{k}.\vec{X}), \qquad 3.3.17$$

where $V(\vec{k})$ is the fourier transform of $W(\vec{X})$. For a Gaussian potential, $V(\vec{k})$ is given by

$$V(\vec{k}) = u^2\eta^2 \exp(-\vec{k}^2L^2/4). \qquad 3.3.18$$

If one inserts (3.3.18) into (3.3.17), one has

$$W[\vec{X}(\tau) - \vec{X}(\sigma)] = u^2\eta^2 \int \frac{d^d\vec{k}}{(2\pi)^d} \exp\left\{-\frac{\vec{k}^2}{4}L^2 + i\vec{k}.[\vec{X}(\tau)-\vec{X}(\sigma)]\right\}. \qquad 3.3.19$$

3.4 Sa-yakanit's Theory

To compute the density of states (3.2.3), the propagator (3.3.12) must be known. However, the propagator (3.3.12) containing the correlation function (3.3.19) is very complicated, and is presently impossible to work out directly. Therefore we must now attack the problem by modeling the correlation function (3.3.19) by some trial actions. Several attempts have been made, and failed[18-22]. Nevertheless, one can obtain an excellent result with a simple one parameter quadratic action. Sa-yakanit is the first to work out a successful theory by modeling the correlation function (3.3.19) with a non-local harmonic oscillator trial action written as follows :

$$S_o(\omega) = \int_o^t d\tau \frac{m}{2}\left\{\dot{\vec{X}}^2(\tau) - \frac{\omega^2}{2t}\int_o^t d\sigma|\vec{X}(\tau) - \vec{X}(\sigma)|^2\right\}, \qquad 3.4.1$$

where ω is a variational parameter to be determined.

We note that the potential part in (3.3.1) is assumed to be non-local. This means that the translational invariance property is built into his formalism, and is also the nature of the disordered system. This property is very important for carrying the calculation. We now rewrite (3.3.12) in the form

$$G(\vec{x}_2,\vec{x}_1;t) = G_o(\vec{x}_2,\vec{x}_1;t)\langle \exp\{\tfrac{i}{\hbar}(S - S_o(\omega))\}\rangle \ , \quad 3.4.2$$

where the non-local harmonic oscillator propagator G_o is given by

$$G_o(\vec{x}_2,\vec{x}_1;t) = \int \mathcal{D}[\vec{x}(\tau)]\exp\{\tfrac{i}{\hbar} S_o(\omega)\} \ , \quad 3.4.3$$

and the average part is regularly defined by

$$\langle Q\rangle = \frac{\int \mathcal{D}[\vec{x}(\tau)]\exp\{i\, S_o(\omega)/\hbar\}Q}{\int \mathcal{D}[\vec{x}(\tau)]\exp\{i\, S_o(\omega)/\hbar\}} \ . \quad 3.4.4$$

The propagator G_o is evaluated exactly in Appendix A, and the average part can be calculated approximately by using the cumulant expansion, as was first pointed out by Kubo[17], that is

$$\langle e^X\rangle = \exp\{\langle X\rangle + \frac{1}{2!}[\langle X^2\rangle - \langle X\rangle^2] + \cdots\}, \quad 3.4.5$$

Moreover, the approximation of the average part approaches to the best estimation by adjusting the variational parameter ω.

Since we are only interested in the difference $(S - S_o)$, the kinetic terms in S and S_o drop out and we only have to consider the reduced actions

$$S_o(\omega) = -\frac{m}{2} \cdot \frac{\omega^2}{2t} \int_o^t \int_o^t d\tau d\sigma |\vec{x}(\tau) - \vec{x}(\sigma)|^2, \qquad 3.4.6$$

$$S = \frac{i}{2\hbar} \bar{N} \int_o^t \int_o^t d\tau d\sigma W[\vec{x}(\tau) - \vec{x}(\sigma)]. \qquad 3.4.7$$

The energy E_o is omitted from (3.4.7) because it can be usually absorbed by the energy E in (3.2.3). However, for the case of the one-dimensional white noise potential, we set $E_o = 0$.

To obtain the density of states, one sets $\vec{x}_2 = \vec{x}_1 = 0$ in (3.4.2) and in (A.8) in Appendix A; we obtain

$$G(o,o;t) = G_o(o,o;t) \langle \exp\{i(S - S_o)/\hbar\} \rangle |_{\vec{x}_2 = \vec{x}_1 = 0}, \qquad 3.4.8$$

$$G_o(o,o;t) = \left(\frac{m}{2\pi i\hbar t}\right)^{d/2} \cdot \left(\frac{\omega t}{2\sin\frac{\omega t}{2}}\right)^{d}. \qquad 3.4.9$$

Substituting (3.4.9) and (3.4.8) into (3.2.3), one finds

$$\rho(E) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt e^{iEt/\hbar} \left(\frac{m}{2\pi i\hbar t}\right)^{d/2} \cdot \left(\frac{\omega t}{2\sin\frac{\omega t}{2}}\right)^{d} \langle \exp\{i(S - S_o)/\hbar\} \rangle , \qquad 3.4.10$$

where the average part is kept in mind that it must be also evaluated by setting $\vec{x}_2 = \vec{x}_1 = 0$.

3.5 First Cumulant Approximation

If the density of states $\rho_1(E)$ depends only on the first cumulant, (3.4.10) reduces to

$$\rho_1(E) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt\left(\frac{m}{2\pi i\hbar t}\right)^{d/2}\cdot\left(\frac{\omega t}{2\sin\frac{\omega t}{2}}\right)^{d}\cdot\exp\{\frac{i}{\hbar}\cdot Et + \frac{i}{\hbar}<S - S_o>\}, \quad 3.5.1$$

where $<S>$ must be worked out directly. For $<S_o>$ we note that

$$\frac{i}{\hbar}<S_o> = [\frac{\partial}{\partial\lambda}\ln G_o(\omega\sqrt{\lambda})]\Big|_{\lambda=1} , \quad 3.5.2$$

where $G_o(\omega\sqrt{\lambda})$ is the usual G_o, with ω replaced by $\omega\sqrt{\lambda}$.

Using (3.4.9), we see that

$$\frac{i}{\hbar}<S_o> = \frac{d}{2}\{1 - \frac{\omega t}{2}\cot\frac{\omega t}{2}\} . \quad 3.5.3$$

For $<S>$ we refer to (2.5.3) and to (C.17) in Appendix C. We get

$$\frac{i}{\hbar}<S> = -\frac{1}{2\hbar^2}\cdot\frac{\xi}{(4\pi)^{d/2}}\cdot t\int_0^t dx j(x,\omega;t)^{-d/2} , \quad 3.5.4$$

where $j(x,\omega;t)$ and x appear in Appendix C by (C.16) and (C.12) respectively. Inserting (3.5.3) and (3.5.4) into (3.5.1), we get

$$\rho_1(E) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt\left(\frac{m}{2\pi i\hbar t}\right)^{d/2}\cdot\left(\frac{\omega t}{2\sin\frac{\omega t}{2}}\right)^{d}\exp\{\frac{i}{\hbar}\cdot Et - \frac{d}{2} + \frac{d}{2}\cdot\frac{\omega t}{2}\cot\frac{\omega t}{2}$$

$$- \frac{1}{2\hbar^2}\cdot\frac{\xi}{(4\pi)^{d/2}}\cdot t\int_0^t dx j(x,\omega;t)^{-d/2}\} \quad 3.5.5$$

According to the uncertainty principle, the limit of ground-state energy implies the limit of large time. If we wish to find the density of states in the ground-state energy, we make the following approximation :

$$\sin\frac{\omega t}{2} \rightarrow \frac{e^{-i\omega t/2}}{2i} , \qquad 3.5.6$$

$$\cot\frac{\omega t}{2} \rightarrow i , \qquad 3.5.7$$

$$\frac{\sin\frac{\omega x}{2}\sin\frac{\omega}{2}(t-x)}{\sin\frac{\omega t}{2}} \rightarrow \frac{1}{2i} . \qquad 3.5.8$$

We now note that in order to obtain (3.5.8) we kept only the leading term of $<S>$ which corresponds to the leading term of $<S_o>$ In this approximation, we have droped out the factor of $e^{-d/2}$ in (3.5.5), and denote the approximate density of states as $\rho_\ell(E)$. Thus (3.5.5) becomes

$$\rho_\ell(E) = \frac{1}{2\pi\hbar}\cdot\int_{-\infty}^{\infty} dt\left(\frac{m\omega}{2\pi\hbar}\right)^{d/2}\cdot(it)^{d/2}\cdot\exp\{-\frac{i}{\hbar}(\frac{d}{4}\cdot E_\omega - E)t - \frac{1}{2\hbar^2}\cdot\frac{\xi}{(4\pi)^{d/2}}\cdot t^2\left(\frac{L}{4}^2 + \frac{\hbar}{2m\omega}\right)^{-d/2}\}, \qquad 3.5.9$$

where $$E_\omega = \hbar\omega . \qquad 3.5.10$$

If $L \rightarrow 0$, then the Gaussian function becomes the Dirac delta function. Consequently, our problem becomes the one-dimensional white noise system when $L \rightarrow 0$ first and $d = 1$,

$$\rho_{\ell}(E) = \frac{1}{2\pi\hbar}\left(\frac{m\omega^2}{2\pi\hbar}\right)^{1/2} \int_{-\infty}^{\infty} dt(it)^{1/2} \cdot \exp\left\{-\frac{i}{\hbar}\left(\frac{E_{\omega}}{4} - E\right)t - \right.$$

$$\left. - \frac{1}{2\hbar^2} \cdot \xi\left(\frac{m\omega}{2\pi\hbar}\right)^{1/2} \cdot t^2 \right\} . \qquad 3.5.11$$

The integral in (3.5.11) can be integrated by using a formula[23]

$$\int_{-\infty}^{\infty} dt(it)^p \exp\{-\beta^2 t^2 - iqt\} = 2^{-p/2}\sqrt{\pi}\,\beta^{-p-1} \exp\left(-\frac{q^2}{8\beta^2}\right) D_p\left(\frac{q}{\beta\sqrt{2}}\right), \qquad 3.5.12$$

where $D_p(z)$ denotes the parabolic cylinder function. If we are interested in the limit of large z, we can use the asymptotic expansion of $D_p(z)$[23]

$$D_p(z) \underset{z \to +\infty}{\approx} \exp\left(-\frac{z^2}{4}\right) z^p . \qquad 3.5.13$$

As pointed out by Halperin and Lax[5], we can reach the low-energy tail by taking the limit $E \to -\infty$ or equivalently the limit $\xi \to 0$. For our case we let $\xi \to 0$, since we are interested in the asymptotic behaviour of the density of states. By defining

$$q = \left(\frac{E_{\omega}}{4} - E\right)/\hbar , \qquad 3.5.14$$

and

$$\beta^2 = \xi\left(\frac{m\omega}{2\pi\hbar}\right)^{1/2}/2\hbar^2 , \qquad 3.5.15$$

and applying (3.5.12) and (3.5.13) to (3.5.11), we find

$$\rho_{\ell}(E) = \frac{1}{2\pi\hbar}\left(\frac{m\omega^2}{2\pi\hbar}\right)^{1/2} 2^{-1/4}\sqrt{\pi}\,\beta^{-3/2} \exp\left(-\frac{q^2}{4\beta^2}\right)\left(\frac{q}{\beta\sqrt{2}}\right)^{1/2} . \qquad 3.5.16$$

As discussed in Chapter II, by taking the limit $\xi \to 0$, we have chosen to maximize the exponential factor in the density of states instead of the density of states. This implies that we must to minimize the exponent of the exponential. Thus when $\xi \to 0$, the exponential factor must be a dominant factor in determining the density of states. This last idea is not based mathematically on the variational principle, and so is useful only in the case of the dominant exponential factor. However, it is easily to minimize the exponent of the exponential in (3.5.16). We begin this procedure by first noting

$$\frac{d}{d\omega}\left(\frac{q^2}{4\beta^2}\right) = 0 \quad , \qquad 3.5.17$$

It follows that

$$E_\omega = -\frac{4}{3}E \, . \qquad 3.5.18$$

The variational equation (3.5.18) is identical to the variational equation which is asymptotically estimated by the Lloyd-Best variational principle[24]. In Appendix F, the equivalent of these two methods will be shown mathematically detail. The proof is rigorous enough to cover the white noise problems in higher dimensions. Inserting (3.5.18) into (3.5.16), we get

$$\rho_\ell(E) = \frac{\sqrt{2\pi}}{6} \cdot \frac{4}{\pi} \cdot \frac{(-E)}{\xi} \cdot \exp\{-(\frac{\pi}{3})^{1/2} \cdot \frac{4\sqrt{2}}{3} \cdot \frac{\hbar}{\sqrt{m}} \cdot \frac{(-E)^{3/2}}{\xi}\} \, . \qquad 3.5.19$$

Comparing (3.5.19) with (1.5.1)

$$\rho_{as}(E) = \frac{4}{\pi} \cdot \frac{(-E)}{\xi} \exp\{-\frac{4\sqrt{2}}{3} \cdot \frac{\hbar}{\sqrt{m}} \cdot \frac{(-E)^{3/2}}{\xi}\} , \qquad 1.5.1$$

we find the agreement between $\rho_{\ell}(E)$ and $\rho_{as}(E)$ to be remarkably good. The powers of E in the exponent and in front of the exponential are correct. The numerical factor in the exponent differs from the exact value by a factor of $(\frac{\pi}{3})^{1/2} = 1.0233$. The numerical factor in front of the exponential is too small by a factor of $\frac{6}{\sqrt{2\pi}} = 2.393$. However, both numerical factors can be improved by going beyond the first cumulant approximation to the second cumulant approximation. In the next chapter, we will find that the numerical factors can be corrected to a great extent by using the complete first cumulant and the leading term approximation in the second cumulant.