

CHAPTER IV

PATH INTEGRAL APPROACH

4.1 Introduction

As was shown by Stern and Hwang,³⁶ the theory of Halperin³⁵ and Lax²⁴ gives reasonable agreement with experiments.

We note however that this theory has three shortcomings. Firstly to obtain the values shown in Table 3.1, one must perform a very complicated calculation using computer which consumes too much time, since they were not able to obtain analytical expression for the density of states.

Secondly, since Halperin and Lax theory makes certain assumptions which restrict its applicability to the deep tail states, it cannot be extended to intermediate states as shown in Fig 4.1.

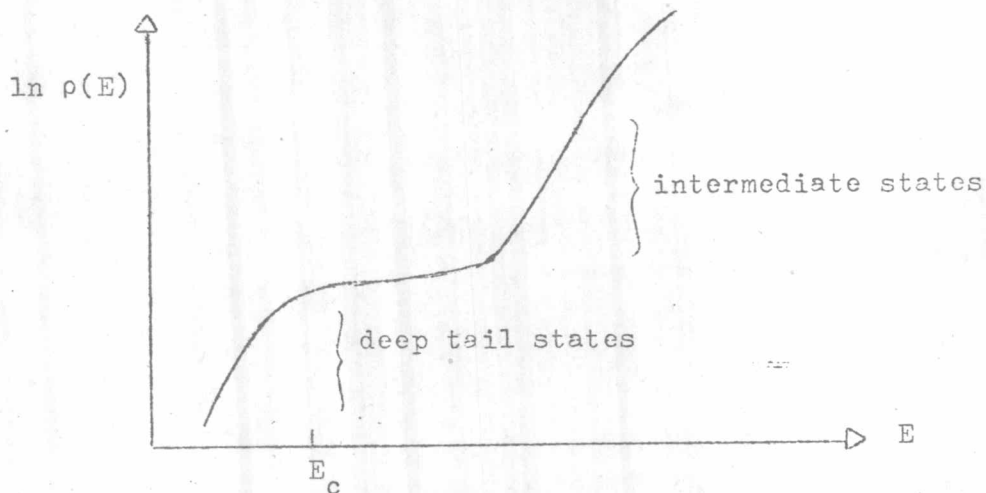


Fig 4.1 Density of states in the tail (schematically)
 E_c is the edge of conduction band.

Thirdly to determine $\rho(E)$, Halperin and Lax maximized the exponential term. This procedure is not valid since it does not base on the variational principle.

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Edwards²⁸ suggested that Path Integral might be used in determining the density of states. Recently Sayakanit applied Path Integral Formalism for calculating the density of states and the effective mass of an electron in Gaussian random system. He proposed that for the three dimensional Gaussian impurity potential, the deep tail states goes approximately as $e^{-B(E)}$ where $B(E)$ is proportional to n with n vary from $\frac{1}{2} \rightarrow 2$. Sayakanit showed also that the method gave the density of states deep in the tail in the form given by Halperin and Lax, however, in analytical forms.

4.2 Path Integral Representation of Green's Function^{27,30,32}

Many properties of electrons can be expressed in terms of the Green's function. For the disordered system, the Green's function to be studied must be the average value of the Green's function.

First we consider the one electron Green's function for an electron in the presence of N scatterers at the fixed positions $\{ \vec{R}_i | i = 1, \dots, N \}$. It should be noted that Green's function must depend on the positions of the scatterers. For the model of N scatterers, the Hamiltonian for the electron is

$$H(\{ \vec{R}_i \}) = -\frac{\hbar^2}{2m} \nabla^2 + \sum_{i=1}^N v(\vec{R}-\vec{R}_i) \quad 4.2.1$$

Since the impurities are randomly distributed, the probability distribution for the scattering centers must be

$$P(\{\vec{R}_i\}) = \frac{1}{\Omega} \prod_{i=1}^N \frac{1}{\pi} d\vec{R}_i \quad 4.2.1$$

where Ω is the volume of the system. For a given configuration of scatterers, we can write the Schrödinger equation for the one electron Green's function as

$$\left[i\hbar \frac{\partial}{\partial t} - H\{\vec{R}_i\} \right] \mathcal{G}(\vec{r}_2, \vec{r}_1; t; \{\vec{R}_i\}) = i\hbar \delta(\vec{r}_1 - \vec{r}_2) \delta(t) \quad 4.2.3$$

Thus the properties of such the system are obtained from the average Green's function $G(\vec{r}_2, \vec{r}_1; t)$, i.e., the average of $\mathcal{G}(\vec{r}_2, \vec{r}_1; t; \{\vec{R}_i\})$ over the random scatterer positions.

The average over all possible configuration $\{\vec{R}_i\}$ is then

$$G(\vec{r}_2, \vec{r}_1; t) = \Omega^{-N} \int \dots \int \prod_{i=1}^N \frac{1}{\pi} d\vec{R}_i \mathcal{G}(\vec{r}_2, \vec{r}_1; t; \{\vec{R}_i\}) \quad 4.2.4$$

The (4.2.3) has the solution $\mathcal{G}(\vec{r}_2, \vec{r}_1; t; \{\vec{R}_i\}) = \langle \vec{r}_2 | e^{-H\{\vec{R}_i\}t/\hbar} | \vec{r}_1 \rangle$ 4.2.5

The time t can be broken up into very short times $(n \cdot \epsilon \rightarrow t)$

$$\mathcal{G}(\vec{r}_2, \vec{r}_1; t; \{\vec{R}_i\}) = \langle \vec{r}_2 | e^{-H\{\vec{R}_i\} \cdot \epsilon / \hbar} e^{-H\{\vec{R}_i\} \cdot \epsilon / \hbar} \dots e^{-H\{\vec{R}_i\} \cdot \epsilon / \hbar} | \vec{r}_1 \rangle$$

$$= \int \dots \int \mathcal{G}(\vec{r}_2, \vec{r}_{n-1}; \epsilon \{\vec{R}_i\}) \dots \mathcal{G}(\vec{r}_2, \vec{r}_1; \epsilon \{\vec{R}_i\}) d\vec{r}_1 \dots d\vec{r}_{n-1} \quad 4.2.7$$

$$= \int D(\vec{r}(\zeta)) \phi(\vec{r}(\zeta)) \quad 4.2.8$$

$$\text{where } D(\vec{r}(\zeta)) = \lim_{n \rightarrow \infty} d\vec{r}_1, d\vec{r}_2 \dots d\vec{r}_n \quad 4.2.9$$

$$\phi(\vec{r}(\zeta)) = \lim_{\epsilon \rightarrow 0} \mathcal{G}(\vec{r}_2, \vec{r}_{n-1}; \epsilon \{\vec{R}_i\}) \dots \mathcal{G}(\vec{r}_2, \vec{r}_1; \epsilon \{\vec{R}_i\}) \quad 4.2.10$$

At very short time ϵ , (4.2.3) can be solved to give

$$\mathcal{G}(\vec{r}_2, \vec{r}_1; \epsilon \{\vec{R}_i\}) \sim \left[\frac{m}{2\pi i \hbar \epsilon} \right]^{3/2} \exp \left\{ \frac{im}{2\hbar \epsilon} (\vec{r}_2 - \vec{r}_1)^2 - \frac{i}{\hbar} \epsilon v \left(\frac{1}{2} (\vec{r}_2 + \vec{r}_1) - \vec{R}_i \right) \right\} \quad 4.2.11$$

This can be substituted into (4.2.10) and then substituted into (4.2.7). The resultant solution is the Feynman path-integral representation of the one electron Green's function.

$$\mathcal{G}(\vec{r}_2, \vec{r}_1; t \{\vec{R}_i\}) = \int_{\vec{r}(0)=\vec{r}_1}^{\vec{r}(t)=\vec{r}_2} D(\vec{r}(\zeta)) \exp \left\{ \frac{i}{\hbar} \cdot \frac{m}{2} \int_0^t d\zeta \dot{\vec{r}}^2(\zeta) - \frac{i}{\hbar} \int_0^t d\zeta \sum_{i=1}^N v(\vec{r}(\zeta) - \vec{R}_i) \right\} \quad 4.2.12$$

where $D(\vec{r}(\zeta))$ is the Feynman measure in configuration space and every path $\vec{r}(\zeta)$ going from $\vec{r}(0) = \vec{r}_1$ to $\vec{r}(t) = \vec{r}_2$. One notes

that the step function is omitted for convenience. The (4.2.12) is now substituted into (4.2.4) and becomes

$$\begin{aligned}
 G(r_2 r_1; t) &= \int_{\vec{r}_2}^{\vec{r}_1} D(\vec{r}(\zeta)) \exp\left[\frac{i}{\hbar} \int_0^t d\zeta \frac{m}{2} \dot{\vec{r}}(\zeta)^2\right] \int \dots \int_{i=1}^N \pi d\vec{R}_i \\
 &\quad \frac{\exp\left[-\frac{i}{\hbar} \int_0^t d\zeta \sum_{i=1}^N v(\vec{r}(\zeta) - \vec{R}_i)\right]}{\Omega^N} \\
 &= \int_{\vec{r}_2}^{\vec{r}_1} D(\vec{r}(\zeta)) \exp\left[\frac{i}{\hbar} \int_0^t d\zeta \frac{m}{2} \dot{\vec{r}}(\zeta)^2\right] \langle \exp\left[-\frac{i}{\hbar} \cdot \right. \\
 &\quad \left. \int_0^t d\zeta \sum_{i=1}^N v(\vec{r}(\zeta) - \vec{R}_i)\right] \rangle_{\{\vec{R}_i\}}
 \end{aligned} \tag{4.2.13}$$

where we define

$$\begin{aligned}
 &\frac{\int \dots \int_{i=1}^N \pi d\vec{R}_i \exp\left[-\frac{i}{\hbar} \int_0^t d\zeta \sum_{i=1}^N v(\vec{r}(\zeta) - \vec{R}_i)\right]}{\Omega^N} \\
 &= \langle \exp\left[-\frac{i}{\hbar} \int_0^t d\zeta \sum_{i=1}^N v(\vec{r}(\zeta) - \vec{R}_i)\right] \rangle_{\{\vec{R}_i\}}
 \end{aligned}$$

Kubo ²⁹ pointed out that the above average $\langle \dots \rangle_{\{\vec{R}_i\}}$

can be rewritten as a cumulant series that is

$$\exp(A\bar{X}) = \sum_{n=0}^{\infty} \frac{A^n m_n}{n!} = \exp \left[\sum_{n=1}^{\infty} \frac{A^n K_n}{n!} \right]$$

where m_n is the n^{th} moment and K_n is the n^{th} cumulant. The relation between K_n and m_n is

$$\frac{K_n}{n!} = \sum_{\{n_i\}} (-1)^{\sum_i n_i - 1} \frac{(\sum_i n_i - 1)!}{i!} \left[\frac{1}{n_i!} \left\{ \frac{m_i}{i!} \right\}^{n_i} \right]$$

Some terms are

$$\begin{aligned} \langle\langle X \rangle\rangle_c &= \langle X \rangle \\ \langle\langle XY \rangle\rangle_c &= \langle XY \rangle - \langle X \rangle \langle Y \rangle \quad \text{etc.} \end{aligned}$$

where c denotes the cumulant series expansion. Using the cumulant series expansion, we have

$$\left\langle \exp \left\{ -\frac{i}{\hbar} \int_0^t d\zeta \sum_{i=1}^N v(\vec{r}(\zeta) - \vec{R}_i) \right\} \right\rangle_{\{\vec{R}\}} = \exp \left\langle \exp \left\{ v(\vec{r}(\zeta) - \vec{R}_1) \right\} - 1 \right\rangle_{c, \{\vec{R}\}}$$

where we define $\sum_i v(\vec{r}(\zeta) - \vec{R}_i)$ as $v(\vec{r}(\zeta) - \{\vec{R}_i\})$ and the symbol

$\langle \rangle_{c, \{\vec{R}\}}$ denotes the cumulant average. Since the random

variables $\{\vec{R}\}$ are statistically independent, so we can write

$$\left\langle \exp \left\{ -\frac{i}{\hbar} \int_0^t d\zeta \sum_{i=1}^N v(\vec{r}(\zeta) - \vec{R}_i) \right\} \right\rangle_{\{\vec{R}\}}$$

$$= \langle \exp \left\{ -\frac{i}{\hbar} \int_0^t d\zeta v(\vec{r}(\zeta) - \vec{R}_1) \right\} \rangle_{\vec{R}_1} \langle \exp \left\{ -\frac{i}{\hbar} \int_0^t d\zeta v(\vec{r}(\zeta) - \vec{R}_2) \right\} \rangle_{\vec{R}_2} \dots$$

4.2.14

As before we can rewrite the average as the cumulant series expansion, we have

$$\begin{aligned} & \langle \exp \left\{ -\frac{i}{\hbar} \int_0^t d\zeta \sum_{i=1}^N v(\vec{r}(\zeta) - \vec{R}_i) \right\} \rangle_{\{\vec{R}\}} \\ &= \exp \left[\langle \exp \left\{ -\frac{i}{\hbar} \int_0^t d\zeta v(\vec{r}(\zeta) - \vec{R}_1) \right\} - 1 \rangle_{c, \vec{R}_1} \right] \\ & \quad \exp \left[\langle \exp \left\{ -\frac{i}{\hbar} \int_0^t d\zeta v(\vec{r}(\zeta) - \vec{R}_2) \right\} - 1 \rangle_{c, \vec{R}_2} \right] \dots \\ &= \exp \left[\langle \exp \left\{ -\frac{i}{\hbar} \int_0^t d\zeta v(\vec{r}(\zeta) - \vec{R}_1) \right\} - 1 \rangle_{c, \vec{R}} \right] \\ & \quad + \langle \exp \left\{ -\frac{i}{\hbar} \int_0^t d\zeta v(\vec{r}(\zeta) - \vec{R}_2) \right\} - 1 \rangle_{c, \vec{R}_2} + \dots \end{aligned} \quad 4.2.15$$

Since $\{\vec{R}\}$ is a set of independent random variables, we can write

$$\langle \exp \left[-\frac{i}{\hbar} \int_0^t d\zeta \sum_{i=1}^N v(\vec{r}(\zeta) - \vec{R}_i) \right] \rangle_{\{\vec{R}\}} = \exp N \langle \exp \left\{ -\frac{i}{\hbar} \int_0^t d\zeta v(\vec{r}(\zeta) - \vec{R}) \right\} - 1 \rangle_{c, \vec{R}} \quad 4.2.16$$

Using the cumulant series expansion the right side of (4.2.16) can be expanded as

$$\exp \left\{ N \left\langle -\frac{i}{\hbar} \int_0^t d\zeta v(\vec{r}(\zeta) - \vec{R}) \right\rangle_c + N \left\langle \frac{1}{2} \left(-\frac{i}{\hbar} \right)^2 \int_0^t \int_0^t d\zeta_1 d\zeta_2 v_1 v_2 \right\rangle_c + \dots \right\}$$

4.2.17

The first term of cumulant series of (4.2.17) can be evaluated as

$$N \left\langle -\frac{i}{\hbar} \int_0^t d\zeta v \right\rangle_c = \left\langle -\frac{i}{\hbar} \int_0^t d\zeta v \right\rangle = -\frac{i}{\hbar} \int_0^t d\zeta \int d\vec{R} v \quad 4.2.18$$

$$= -\frac{i}{\hbar} \int_0^t E_0 d\zeta, \text{ where } E_0 = n \int d\vec{R} v = \text{constant}.$$

4.2.19

The second term of cumulant series of (4.2.17) can be written as

$$N \left\langle \frac{1}{2} \left(-\frac{i}{\hbar} \right)^2 \int_0^t \int_0^t d\zeta_1 d\zeta_2 v_1 v_2 \right\rangle_c = \frac{N}{2} \left(-\frac{i}{\hbar} \right)^2 \left\{ \left(\int_0^t \frac{d\vec{R}}{\Omega} \left(\int_0^t d\zeta_1 v_1 \right)^2 - \left(\int_0^t \frac{d\vec{R}}{\Omega} \int_0^t d\zeta_1 v_1 \right)^2 \right\} \quad 4.2.20$$

As $\Omega \rightarrow \infty$ the second term on the right hand side can be neglected

and we get

$$N \left\langle \frac{1}{2} \left(-\frac{i}{\hbar} \right)^2 \int_0^t \int_0^t d\zeta_1 d\zeta_2 v_1 v_2 \right\rangle_c = \frac{N}{2} \left(-\frac{i}{\hbar} \right)^2 \int_0^t \frac{d\vec{R}}{\Omega} \left(\int_0^t d\zeta v \right)^2 \quad 4.2.21$$

Using the same argument, we can show that when $\Omega \rightarrow \infty$, one should keep the first term of each cumulant. Then (4.2.20) becomes

$$G(\vec{r}_2, \vec{r}_1; t) = \frac{\int_{r_1}^{r_2} D(\vec{r}(\zeta)) e^{\frac{i}{\hbar}(S - S_0)} e^{\frac{i}{\hbar}S_0} \cdot G_0(\vec{r}_2, \vec{r}_1; t)}{\int_{r_1}^{r_2} D(\vec{r}(\zeta)) e^{\frac{i}{\hbar}S_0}}$$

Thus $G(\vec{r}_2, \vec{r}_1; t) = \langle \exp \frac{i}{\hbar}(S - S_0) \rangle_{S_0} G_0(\vec{r}_2, \vec{r}_1; t)$ 4.2.27

Then $\langle \exp \frac{i}{\hbar}(S - S_0) \rangle_{S_0}$ is expanded in cumulant series

$$\langle e^{\frac{i}{\hbar}(S - S_0)} \rangle_{S_0} = \exp \left(\frac{i}{\hbar} \langle S - S_0 \rangle_{S_0} + \frac{1}{2} \left(\frac{i}{\hbar} \right)^2 \right.$$

$$\left. \left(\langle (S - S_0)^2 \rangle_{S_0} - \langle S - S_0 \rangle_{S_0}^2 \right) + \dots \right) \quad 4.2.28$$

where $\langle (S - S_0)^n \rangle_{S_0} = \frac{\int (S - S_0)^n e^{-S_0} D \vec{r}(\zeta)}{\int e^{-S_0} D \vec{r}(\zeta)}$

For solving $G_0(\vec{r}_2, \vec{r}_1; t)$ and $\langle S - S_0 \rangle$, a trial action must be a non-local harmonic action $S_0(\omega)$

4.3 The evaluation of $G_0(\vec{r}_2, \vec{r}_1; t)$ ³⁰

Sayakanit (1974) has introduced the following trial action

$$S_0(\omega) = \int_0^t d\zeta \frac{m}{2} \left\{ \dot{\vec{r}}^2(\zeta) - \frac{1}{2t} \omega^2 \int_0^t d\sigma |\vec{r}(\zeta) - \vec{r}(\sigma)|^2 \right\} \quad 4.3.1$$

$$\begin{aligned}
& \exp \left(1 + n \left(-\frac{i}{\hbar} \right) \int_0^t d\vec{R} \left(\int_0^t v d\zeta + \frac{n}{2} \left(-\frac{i}{\hbar} \right)^2 \int_0^t d\vec{R} \left[\int_0^t v d\zeta \right]^2 + \right. \right. \\
& \quad \left. \left. \dots + \frac{n}{m!} \left(-\frac{i}{\hbar} \right)^m \int_0^t d\vec{R} \cdot \left(\int_0^t d\zeta v \right)^m + \dots - 1 \right) \right) \\
& = \exp \left\{ \frac{n}{\hbar} \int_0^t d\vec{R} \left(\exp \left(-\frac{i}{\hbar} \int_0^t v d\zeta \right) - 1 \right) \right\} \tag{4.2.22}
\end{aligned}$$

where $\sum_{k=0}^{\infty} \frac{x^k}{k!} = e^x$

Substituting (4.2.22) into (4.2.15), the Green's function becomes

$$\begin{aligned}
G(\vec{r}_2, \vec{r}_1, t) &= \int_{\vec{r}_1}^{\vec{r}_2} D(\vec{r}(\zeta)) \exp \left[\frac{i}{\hbar} \int_0^t d\zeta \frac{m}{2} \dot{\vec{r}}^2(\zeta) + \right. \\
& \quad \left. + n \int_0^t d\vec{R} \left(\exp \left(-\frac{i}{\hbar} \int_0^t v(\vec{r}(\zeta) - \vec{R}) d\zeta \right) - 1 \right) \right] \tag{4.2.23}
\end{aligned}$$

Since we consider in the limit ($n \rightarrow \infty$, $v \rightarrow 0$, nv^2 finite), and so we keep only the first two terms in the series expansions of the interaction term are required. We use (4.2.20) and (4.2.21), (4.2.23) becomes

$$\begin{aligned}
G(\vec{r}_2, \vec{r}_1, t) &= \int_{\vec{r}(0)=\vec{r}_1}^{\vec{r}(t)=\vec{r}_2} D(\vec{r}(\zeta)) \left\{ \exp \left[\frac{i}{\hbar} \frac{m}{2} \int_0^t d\zeta \dot{\vec{r}}^2(\zeta) - \frac{i}{\hbar} \int_0^t d\zeta E_0 \right. \right. \\
& \quad \left. \left. + \frac{n}{2} \left(-\frac{i}{\hbar} \right)^2 \int_0^t d\zeta \int_0^t d\sigma v(\vec{r}(\zeta) - \vec{R}) v(\vec{r}(\sigma) - \vec{R}) \right] \right\}
\end{aligned}$$

$$\begin{aligned}
= & \int_{\vec{r}_1}^{\vec{r}_2} D(\vec{r}(\zeta)) \exp \left\{ \frac{i}{\hbar} \frac{m}{2} \int_0^t d\zeta \dot{\vec{r}}^2(\zeta) - \frac{i}{\hbar} E_0 t \right. \\
& \left. - \frac{n}{2\hbar^2} \int_0^t d\zeta \int_0^t d\sigma W(\vec{r}(\zeta) - \vec{r}(\sigma)) \right\}
\end{aligned} \tag{4.2.24}$$

$$\text{where } W(\vec{r}) = \int \frac{d^3\vec{k}}{(2\pi)^3} \exp(i\vec{k} \cdot \vec{r}) v_k^2$$

and v_k is the Fourier transform of $v(\vec{r})$.

G can be considered to describe the propagation of the particle, and $\vec{r}(\zeta)$ describes the average electron's path with the self energy $W(\vec{r}(\zeta) - \vec{r}(\sigma))$.

To solve $G(\vec{r}_2, \vec{r}_1; t)$ we use the variational method. We introduce

$$G_0(\vec{r}_2, \vec{r}_1; t) = \int_{\vec{r}_1}^{\vec{r}_2} D(\vec{r}(\zeta)) e^{i/\hbar S_0(\vec{r}(\zeta))} \tag{4.2.25}$$

where $S_0(\vec{r}(\zeta))$ is the trial action chosen so that G_0 can be worked out, and

$$G(\vec{r}_2, \vec{r}_1; t) = \int_{\vec{r}_1}^{\vec{r}_2} D(\vec{r}(\zeta)) e^{i/\hbar S(\vec{r}(\zeta))} \tag{4.2.26}$$

Then $G(\vec{r}_2, \vec{r}_1; t)$ can be approximately solved by using the variational principle for path integration with which the trial action S_0 containing some parametrized form for the potential and varying the parameter.

where ω is an adjustable parameter. Then G_0 can be written as

$$G_0(\vec{r}_2, \vec{r}_1; t) = \int_{\vec{r}_1}^{\vec{r}_2} D(\vec{r}(\zeta)) \exp\left[\frac{i}{\hbar} \int_0^t d\zeta \frac{m}{2} \dot{\vec{r}}^2(\zeta) - \frac{1}{2t} \omega^2 \int_0^t d\sigma |\vec{r}(\zeta) - \vec{r}(\sigma)|^2\right]$$

4.3.2

Since

$$\langle Q \rangle_{\vec{R}} = \frac{\int d\vec{R} e^{i/\hbar R^2} Q(\{\vec{R}\})}{\int d\vec{R} e^{i/\hbar R^2}}$$

Then

$$e^{\frac{i}{\hbar} \frac{m}{2} \frac{\omega^2}{t} \int_0^t \int_0^t d\zeta d\sigma \vec{r}(\zeta) \cdot \vec{r}(\sigma)} = \frac{\int d\vec{R} e^{i/\hbar R^2 + \frac{i}{\hbar} \omega \sqrt{\frac{2m}{t}} \int_0^t d\zeta \vec{r}(\zeta) \cdot \vec{R}}}{\int d\vec{R} e^{i/\hbar R^2}}$$

where

$$\int_{-\infty}^{\infty} e^{ax^2 + bx} dx = \sqrt{\frac{\pi}{-a}} e^{-b^2/4a}$$

Therefore

$$G_0(\vec{r}_2, \vec{r}_1; t) = \frac{\int d\vec{R} e^{i/\hbar R^2} \int_{\vec{r}_2}^{\vec{r}_1} D(\vec{r}(\zeta)) e^{\frac{i}{\hbar} \int_0^t d\zeta \left(\frac{m}{2} \dot{\vec{r}}^2(\zeta) - \frac{m}{2} \omega^2 \vec{r}(\zeta) \cdot \omega \sqrt{\frac{2m}{t}} \vec{r}(\zeta) \cdot \vec{R} \right)}}{\int d\vec{R} e^{i/\hbar R^2}} \quad 4.3.3$$

$$= \langle G_0(\vec{r}_2, \vec{r}_1; t) \{ \vec{R} \} \rangle_{\vec{R}}$$

where $G_0(\vec{r}_2, \vec{r}_1; t) \{ \vec{R} \} = \int_{\vec{r}_1}^{\vec{r}_2} D(\vec{r}(\zeta)) e^{\frac{i}{\hbar} \int_0^t d\zeta \left(\frac{m}{2} \dot{\vec{r}}^2(\zeta) - \frac{m}{2} \omega^2 \vec{r}(\zeta) \cdot \omega \sqrt{\frac{2m}{t}} \vec{r}(\zeta) \cdot \vec{R} \right)}$

The solution of $G_0(\vec{r}_2, \vec{r}_1; t | \vec{R})$ is compared to the well known solution of forced harmonic oscillator and has the form

$$\begin{aligned}
 G_0(\vec{r}_2, \vec{r}_1; t | \vec{R}) = & \left(\frac{m\omega}{2\pi i \hbar \sin \omega t} \right)^{1/2} \exp \frac{i}{\hbar} \left[\frac{m\omega}{2 \sin \omega t} (\vec{r}_2 + \vec{r}_1)^2 \cos \omega t \right. \\
 & - 2\vec{r}_1 \cdot \vec{r}_2 + \frac{2}{m\omega} \vec{r}_2 \cdot \vec{R} \int_0^t d\zeta \omega \sqrt{\frac{2m}{t}} \sin \omega \zeta \\
 & + \frac{2\vec{r}_1 \cdot \vec{R}}{m\omega} \int_0^t d\zeta \omega \sqrt{\frac{2m}{t}} \sin \omega (t - \zeta) \\
 & \left. - \frac{2}{m^2 \omega^2} \vec{R}^2 \int_0^t d\zeta \omega \sqrt{\frac{2m}{t}} \sin \omega (t - \zeta) \int_0^t d\sigma \omega \sqrt{\frac{2m}{t}} \sin \omega \sigma \right]
 \end{aligned}$$

4.3.4

Substituting (4.3.4) into (4.3.3) and performing integration with respect to \vec{R} , we get

$$G_0(\vec{r}_2, \vec{r}_1; t) = \left(\frac{m}{2\pi i \hbar t} \right)^{3/2} \left(\frac{\omega t}{2 \sin \frac{\omega t}{2}} \right)^3 \exp \left\{ \frac{i}{\hbar} \frac{m\omega}{4} \cot \frac{\omega t}{2} |\vec{r}_2 - \vec{r}_1|^2 \right\} \quad 4.3.5$$

4.4 The Evaluation of $\langle S - S_0 \rangle_{S_0}$ 30,32

If $\langle S - S_0 \rangle_{S_0}$ is small, we need to keep the first cumulant of (4.2.28). Thus we have

$$\begin{aligned}
\langle S - S_0 \rangle_{S_0} &= \langle \frac{i}{2\hbar} n \int_0^t \int d\zeta d\sigma W(\vec{r}(\zeta) - \vec{r}(\sigma)) + \frac{m\omega^2}{4t} \int_0^t \int d\zeta d\sigma |\vec{r}(\zeta) - \vec{r}(\sigma)|^2 \rangle_{S_0} \\
&= \frac{i n}{2\hbar} \int_0^t \int d\zeta d\sigma \langle W(\vec{r}(\zeta) - \vec{r}(\sigma)) \rangle + \frac{m\omega^2}{4t} \int_0^t \int d\zeta d\sigma \langle |\vec{r}(\zeta) - \vec{r}(\sigma)|^2 \rangle_{S_0}
\end{aligned}$$

4.4.1

To solve (4.4.1), $W(\vec{r}(\zeta) - \vec{r}(\sigma))$ must be considered. In case of heavily doped semiconductors, the impurity potential is in the form

$$v(\vec{r}(\zeta) - \vec{R}) = \frac{-Ze^2}{\epsilon} \frac{\exp(-Q|\vec{r}(\zeta) - \vec{R}|)}{|\vec{r}(\zeta) - \vec{R}|} \quad 4.4.2$$

The Fourier transform of $W(\vec{r}(\zeta) - \vec{r}(\sigma))$ is

$$\begin{aligned}
W(\vec{r}(\zeta) - \vec{r}(\sigma)) &= \int d\vec{R} v(\vec{r}(\zeta) - \vec{R}) v(\vec{r}(\sigma) - \vec{R}) \\
&= (2\pi)^{-3} \int d\vec{R} \left(v_{\vec{k}} e^{-i\vec{k} \cdot (\vec{r}(\zeta) - \vec{R})} \right. \\
&\quad \left. \int d^3\vec{k} v_{\vec{J}} e^{i\vec{J} \cdot (\vec{r}(\sigma) - \vec{R})} \int d^3\vec{J} \right)
\end{aligned}$$

where $v_{\vec{k}}$ and $v_{\vec{J}}$ is the Fourier transform of the potential.

Partially evaluating the above equation, we have

$$W(\vec{r}(\zeta) - \vec{r}(\sigma)) = (2\pi)^{-3} \int v_{\vec{k}} v_{\vec{J}} e^{-i(\vec{k} \cdot \vec{r}(\zeta) + \vec{J} \cdot \vec{r}(\sigma))} d^3\vec{k} d^3\vec{J} \int d\vec{R} e^{i(\vec{k} + \vec{J}) \cdot \vec{R}}$$

$$\begin{aligned}
&= (2\pi)^{-3} \int v_{\vec{k}} v_{\vec{J}} e^{-i(\vec{k} \cdot \vec{r}(\zeta) + \vec{J} \cdot \vec{r}(\sigma))} d^3_{\vec{k}} d^3_{\vec{J}} (2\pi)^3 \delta(\vec{k} + \vec{J}) \\
&= \int |v_{\vec{k}}|^2 e^{i\vec{k} \cdot (\vec{r}(\zeta) - \vec{r}(\sigma))} d^3_{\vec{k}} \tag{4.4.3}
\end{aligned}$$

Taking the Fourier transform of (4.4.2), we get

$$\begin{aligned}
v_{\vec{k}} &= \frac{-Ze^2}{\epsilon} \frac{1}{(2\pi)^{3/2}} \int \frac{d^3_{\vec{r}}}{r} e^{-Qr} e^{-i\vec{k} \cdot \vec{r}} \\
&= \frac{-Ze^2}{\epsilon} \frac{1}{(2\pi)^{3/2}} 2\pi \int_0^\infty r dr \int_{-1}^1 d\mu e^{-Qr - i\vec{k} \cdot \vec{r}} \\
&= \frac{-Ze^2}{\epsilon} \frac{1}{(2\pi)^{3/2}} \left(\frac{4\pi}{k^2 + Q^2} \right)
\end{aligned}$$

Substituting the above result into (4.4.3), and taking the average

$$\text{we obtain } \langle W(\vec{r}(\zeta) - \vec{r}(\sigma)) \rangle = \frac{\xi}{n} \frac{Q}{2\pi} \int \frac{d^3_{\vec{k}}}{(2\pi)^3} \left(\frac{4\pi}{k^2 + Q^2} \right)^2 \langle e^{i\vec{k} \cdot (\vec{r}(\zeta) - \vec{r}(\sigma))} \rangle \tag{4.4.4}$$

$$\text{where } \xi = \frac{2\pi Z^2 e^4 n}{Q \epsilon^2} \tag{4.4.5}$$

$\langle e^{i\vec{k} \cdot (\vec{r}(\zeta) - \vec{r}(\sigma))} \rangle$ can be expanded in cumulant series, and keep S_0

only the first two terms, the other terms are zero since S_0 is

quadratic, we obtain $\langle \exp(i\vec{k} \cdot (\vec{r}(\zeta) - \vec{r}(\sigma))) \rangle_{S_0}$

$$= \exp \left\{ i\vec{k} \cdot \langle \vec{r}(\zeta) - \vec{r}(\sigma) \rangle_{S_0} + \frac{i^2 k^2}{2} \left(\frac{1}{3} \langle (\vec{r}(\zeta) - \vec{r}(\sigma))^2 \rangle - \frac{1}{3} \langle \vec{r}(\zeta) - \vec{r}(\sigma) \rangle^2 \right) \right\} \quad 4.4.6$$

One notes that $\vec{k} \cdot \vec{r} = \frac{1}{3} kr$.

From (4.4.6) one notes that $\vec{r}_c(\zeta)$ must be evaluated.

The characteristic functional is defined as

$$\langle e^{\frac{i}{\hbar} \int_0^t d\zeta f(\zeta) \cdot \vec{r}(\zeta)} \rangle_{S_0} = \int_{r_1}^{r_2} \underbrace{D(\vec{r}(\zeta)) e^{\frac{i}{\hbar} S_0}}_{r_1} \cdot e^{\frac{i}{\hbar} \int_0^t d\zeta f(\zeta) \cdot \vec{r}(\zeta)} \quad 4.4.7$$

$$\text{Let } S' = S_0 + \int_0^t d\zeta f(\zeta) \cdot \vec{r}(\zeta) \quad 4.4.8$$

Let us define $\vec{r}_c(\zeta) + \vec{y}(\zeta) = \vec{r}(\zeta)$ where $\vec{r}_c(\zeta)$ is the classical path corresponding to the extremum of the action S . If the S_c is the extremum of the action S then the factor $e^{\frac{i}{\hbar} S_c}$ can be

extracted as a factor of the path integral of (4.4.7) (one lets $\vec{r}(\zeta) = \vec{r}_c(\zeta) + \vec{y}(\zeta)$). The remaining factor is a path integral



over the path $y(\zeta)$ which runs from (0 to 0) and the integral over the path $y(\zeta)$ does not depend upon the function $f(\zeta)$.

Substituting ; $\vec{r}_c(\zeta) + \vec{y}(\zeta) = \vec{r}(\zeta)$ in (4.4.7) one gets

$$\begin{aligned}
 \left\langle e^{\frac{i}{\hbar} \int_0^t d\zeta f(\zeta) \cdot \vec{r}(\zeta)} \right\rangle_{S_0} &= \frac{e^{\frac{i}{\hbar} S_c} \int_{\vec{y}(0)=0}^{\vec{y}(t)=0} D(\vec{y}(\zeta)) \exp\left\{ \frac{i}{\hbar} \int_0^t d\zeta \vec{y}(\zeta) \cdot f(\zeta) \right\}}{e^{\frac{i}{\hbar} S_{0,c}} \int_{\vec{y}(0)=0}^{\vec{y}(t)=0} D(\vec{y}(\zeta)) \exp\left\{ \frac{i}{\hbar} S_0 \right\}} \\
 &= \exp \left\{ \frac{i}{\hbar} (S'_c - S_{0,c}) \right\} \qquad 4.4.9
 \end{aligned}$$

where $S_{0,c}$ is the extremum of action S_0 . The functional derivatives can be obtained as follows

$$\begin{aligned}
 \frac{\delta}{\delta f} \left\langle e^{\frac{i}{\hbar} \int_0^t f(\zeta) \cdot \vec{r}(\zeta)} \right\rangle_{S_0} &= \frac{\delta}{\delta f} e^{\frac{i}{\hbar} (S'_c - S_{0,c})} \\
 \left\langle \vec{r}(\zeta) e^{\frac{i}{\hbar} \int_0^t f(\zeta) \cdot \vec{r}(\zeta)} \right\rangle_{S_0, f=0} &= \frac{\delta S_c}{\delta f} e^{\frac{i}{\hbar} (S'_c - S_{0,c})} \Big|_{f=0} \qquad 4.4.10
 \end{aligned}$$

Eq.(4.4.9) can be differentiated with respect to $f(\zeta)$ and $f(\sigma)$ respectively, to become

$$\left\langle \vec{r}(\zeta) \vec{r}(\sigma) \right\rangle_{S_0} = \left\{ \frac{\hbar}{i} \frac{\delta^2 S'_c}{\delta f(\zeta) \delta f(\sigma)} + \frac{\delta S'_c}{\delta f(\zeta)} \cdot \frac{\delta S'_c}{\delta f(\sigma)} \right\} \Big|_{f=0} \qquad 4.4.11$$

If one lets $\zeta = \sigma$, (4.4.51) becomes

$$\langle \vec{r}^2(\zeta) \rangle_{S_0} = \left. \left\{ \frac{\hbar \delta^2 S'_c}{i \delta f(\zeta) \delta f(\sigma)} \Big|_{\zeta=\sigma} + \frac{\delta S'_c}{\delta f(\zeta)} \frac{\delta S'_c}{\delta f(\sigma)} \Big|_{\zeta=\sigma} \right\} \right|_{f=0} \quad 4.4.12$$

To solve the classical action S'_c , we begin with

$$S' = \frac{m}{2} \int_0^t d\zeta \dot{\vec{r}}^2(\zeta) - \frac{m\omega^2}{4t} \int_0^t d\zeta \int_0^t d\sigma |\vec{r}(\zeta) - \vec{r}(\sigma)|^2 + \int_0^t f(\zeta) \cdot \vec{r}(\zeta) d\zeta \quad 4.4.13$$

The extremum of S' is S'_c which can be found by the prescription

$$\begin{aligned} \delta S' &= m \int_0^t \dot{\vec{r}}(\zeta) \delta(\vec{r}(\zeta)) d\zeta - \frac{2m\omega^2}{4t} \int_0^t \int_0^t (\vec{r}(\zeta) - \vec{r}(\sigma)) \delta(\vec{r}(\zeta) - \vec{r}(\sigma)) d\zeta d\sigma \\ &\quad + \int_0^t f(\zeta) \delta \vec{r}(\zeta) d\zeta \\ &= 0 \end{aligned}$$

Then one make the integration by part of the first term and rearrange the second term

$$\begin{aligned} \delta S' &= m \dot{\vec{r}}(\zeta) \delta(\vec{r}(\zeta)) \Big|_0^t - m \int_0^t \dot{\vec{r}}(\zeta) \delta \vec{r}(\zeta) d\zeta + m\omega^2 \int_0^t \vec{r}(\zeta) \delta(\vec{r}(\zeta)) d\zeta \\ &\quad - \frac{m\omega^2}{t} \int_0^t \int_0^t d\zeta d\sigma \vec{r}(\zeta) \delta(\vec{r}(\zeta)) d\zeta + \int_0^t f(\zeta) \delta(\vec{r}(\zeta)) d\zeta \\ &= 0 \end{aligned}$$

One obtains the classical equation

$$d^2 \vec{r}_c(\zeta) + \omega^2 \vec{r}_c(\zeta) = \frac{f(\zeta)}{m} + \frac{\omega^2}{t} \int_0^t d\sigma \vec{r}_c(\sigma) \quad 4.4.14$$

This can be solved by introducing

$$\left(\frac{d^2}{d\zeta^2} + \omega^2 \right) g(\zeta, \sigma) = \delta(\zeta - \sigma) \quad 4.4.15$$

where

$$g(\zeta, \sigma) = \frac{1}{\omega \sin \omega t} \left(\sin \omega(t - \sigma) \sin \omega \zeta H(\sigma - \zeta) \right. \\ \left. + \sin \omega \sigma \sin \omega(t - \zeta) H(\zeta - \sigma) \right) \quad 4.4.16$$

and

$$H(X) = \begin{cases} 1 & X > 0 \\ 0 & X < 0 \end{cases}$$

Multiplying (4.4.15) by $\vec{r}_c(\zeta)$ and (4.4.14) by $g(\zeta, \sigma)$ then subtracting and integrating from 0 to t , one obtains

$$\begin{aligned} \vec{r}_c(\sigma) &= \int_0^t \frac{\omega^2}{t} \int_0^t d\zeta d\sigma g(\zeta, \sigma) \vec{r}_c(\zeta) + \int_0^t g(\zeta, \sigma) \frac{f(\zeta)}{m} d\zeta + \vec{r}_c(\zeta) \left. \frac{d}{d\zeta} g(\zeta, \sigma) \right|_0^t \\ &= \int_0^t \frac{\omega^2}{t} \int_0^t g(\zeta, \sigma) \vec{r}_c(\sigma) d\sigma d\zeta + \int_0^t g(\zeta, \sigma) \frac{f(\zeta)}{m} d\zeta \\ &\quad + \left(\vec{r}_c(t) \frac{\sin \omega \sigma}{\sin \omega t} + \frac{\vec{r}_c(0) \sin \omega(t - \sigma)}{\sin \omega t} \right) \end{aligned}$$

$$\begin{aligned} \vec{r}_c(\sigma) = & \frac{1}{\sin \omega t} (\vec{r}_2 \sin \omega \sigma + \vec{r}_1 \sin \omega (t - \sigma)) + \frac{1}{t^2} \int_0^t \vec{r}_c(\sigma) d\sigma \int_0^t g(\zeta, \sigma) d\zeta \\ & + \frac{1}{m} \int_0^t g(\zeta, \sigma) f(\zeta) d\zeta \end{aligned} \quad 4.4.17$$

where $\vec{r}_1 = \dot{\vec{r}}_c(0)$, $\vec{r}_2 = \dot{\vec{r}}_c(t)$

Then
$$\int_0^t \vec{r}_c(\sigma) d\sigma = \frac{1}{\sin \omega t} \int_0^t (\vec{r}_2 \sin \omega \sigma + \vec{r}_1 \sin \omega (t - \sigma)) d\sigma$$

$$+ \int_0^t \frac{1}{t^2} \vec{r}_c(\sigma) d\sigma \int_0^t \int_0^t g(\zeta, \sigma) d\sigma d\zeta$$

$$+ \frac{1}{m} \int_0^t \int_0^t g(\zeta, \sigma) f(\zeta) d\zeta d\sigma$$

$$\begin{aligned} \int_0^t \vec{r}_c(\sigma) d\sigma - \frac{1}{t^2} \int_0^t \vec{r}_c(\sigma) d\sigma \int_0^t \int_0^t g(\zeta, \sigma) d\sigma d\zeta \\ = \frac{1}{\sin \omega t} \int_0^t (\vec{r}_2 \sin \omega \sigma + \vec{r}_1 \sin \omega (t - \sigma)) d\sigma \\ + \frac{1}{m} \int_0^t \int_0^t g(\zeta, \sigma) f(\zeta) d\zeta d\sigma. \end{aligned}$$

$$\int_0^t \vec{r}_c(\zeta) d\sigma =$$

$$\frac{1}{\sin \omega t} \int_0^t (\vec{r}_2 \sin \omega \sigma + \vec{r}_1 \sin \omega (t - \sigma)) d\sigma + \frac{1}{m} \int_0^t \int_0^t g(\zeta, \sigma) f(\zeta) d\zeta d\sigma$$

$$1 - \frac{\omega^2}{t^2} \int_0^t \int_0^t g(\zeta, \sigma) d\zeta d\sigma$$

$$\int_0^t g(\zeta, \sigma) d\zeta = \int_0^\sigma g(\zeta, \sigma) d\zeta + \int_\sigma^t g(\zeta, \sigma) d\zeta$$

$$= -\frac{4}{\omega^2} \sin \frac{\omega}{2} \sigma \sin \frac{\omega}{2} (t-\sigma) \sin \frac{\omega t}{2} / \sin \omega t$$

$$\int_0^t \int_0^t g(\zeta, \sigma) d\zeta d\sigma = -\frac{2}{\omega} \left(\frac{1}{\omega} \tan \frac{\omega t}{2} - \frac{t}{2} \right)$$

$$\int_0^t \sin \omega \sigma d\sigma = \frac{1}{\omega} (1 - \cos \omega t) = \frac{2}{\omega} \sin^2 \frac{\omega t}{2}$$

$$= \int_0^t \sin \omega (t-\sigma) d\sigma$$

Substituting the above into (4.4.18) one obtains

$$\int_0^t \dot{r}_c(\sigma) d\sigma = \left(\frac{r_2 + r_1}{2} \right) \frac{t}{2} - \frac{2t}{m\omega} \int_0^t d\sigma f(\zeta) \sin \frac{\omega \sigma}{2} \sin \frac{\omega}{2} (t-\sigma) \cos \frac{\omega t}{2} / \sin \omega t$$

4.4.19

Eq. 4.4.19 can be substituted into (4.4.17) and (4.4.17) becomes

$$r_c(\zeta) = \frac{1}{\sin \omega t} \left[r_2 \sin \omega \zeta + r_1 \sin \omega (t-\zeta) - 4 \sin \frac{1}{2} \omega (t-\zeta) \sin \frac{1}{2} \omega \zeta \right.$$

$$\left. \sin \frac{\omega t}{2} \left\{ \left(\frac{r_2 + r_1}{2} \right) \frac{1}{2} - \frac{2}{m\omega \sin \omega t} \int_0^t d\sigma f(\sigma) \sin \frac{1}{2} \omega \sigma \sin \frac{1}{2} \omega (t-\sigma) \right. \right.$$

$$\left. \left. \cos \frac{\omega t}{2} \right\} \right] + \frac{1}{m} \int_0^t d\sigma f(\sigma) g(\zeta, \sigma) \quad 4.4.20$$

$$\begin{aligned} \vec{r}_c(\zeta) = & \frac{1}{\sin \omega t} \left[\vec{r}_2 \sin \omega \zeta + \vec{r}_1 \sin (t-\zeta) - 4 \sin \frac{1}{2} \omega (t-\zeta) \sin \frac{\omega \zeta}{2} \right. \\ & \left. \left\{ \frac{1}{2} (\vec{r}_2 + \vec{r}_1) \sin \frac{\omega}{2} - \frac{1}{m \omega} \int_0^t d\sigma f(\sigma) \sin \frac{1}{2} \omega \sigma \sin \frac{1}{2} \omega (t-\sigma) \right\} \right] \\ & + \frac{1}{m} \int_0^t d\sigma f(\sigma) g(\zeta, \sigma) \end{aligned} \quad 4.4.21$$

Then multiplying $\vec{r}_c(\zeta)$ by $f(\zeta)$ and integrating from 0 to t , we get

$$\begin{aligned} \int_0^t f(\zeta) \cdot \vec{r}_c(\zeta) d\zeta = & \frac{1}{\sin \omega t} \left\{ \vec{r}_2 \int_0^t f(\zeta) \sin \omega \zeta d\zeta + \vec{r}_1 \int_0^t f(\zeta) \sin \omega (t-\zeta) d\zeta \right. \\ & - \vec{r}_2 \int_0^t d\zeta f(\zeta) \cdot 2 \cdot \frac{\sin \omega (t-\zeta)}{2} \sin \frac{\omega \zeta}{2} \sin \frac{\omega t}{2} \\ & - \vec{r}_1 \int_0^t d\zeta f(\zeta) \cdot 2 \cdot \frac{\sin \omega (t-\zeta)}{2} \sin \frac{\omega \zeta}{2} \sin \frac{\omega t}{2} \\ & + \frac{4}{m \omega} \int_0^t \int_0^t d\zeta d\sigma f(\zeta) \cdot f(\sigma) \sin \frac{1}{2} \omega (t-\zeta) \sin \frac{\omega}{2} \zeta \sin \frac{\omega}{2} (t-\sigma) \\ & \left. \cdot \sin \frac{1}{2} \omega \sigma \right\} + \frac{1}{m} \int_0^t \int_0^t d\zeta d\sigma f(\zeta) f(\sigma) g(\zeta, \sigma) \end{aligned}$$

Considering the case of $\zeta > \sigma$ where $g(\zeta, \sigma) = \frac{-\sin \omega (t-\zeta) \sin \omega \sigma}{\omega \sin \omega t}$

and where there is a symmetry of ζ and σ , one can replace

$$\int_0^t \int_0^t d\zeta d\sigma F(\zeta, \sigma) \text{ by } 2 \int_0^t \int_0^\zeta d\zeta d\sigma F(\zeta, \sigma), \text{ to get}$$

$$\begin{aligned}
\int_0^t f(\zeta) \cdot \vec{r}_c(\zeta) d\zeta &= \frac{1}{\sin \omega t} \left[\frac{1}{2} \int_0^t f(\zeta) d\zeta \left\{ \sin \omega \zeta - 2 \sin \frac{\omega}{2}(t-\zeta) \sin \frac{\omega}{2} \zeta \sin \frac{\omega t}{2} \right\} \right. \\
&\quad \left. + \vec{r}_1 \int_0^t f(\zeta) d\zeta \left\{ \sin \omega(t-\zeta) - 2 \sin \frac{\omega}{2}(t-\zeta) \sin \frac{\omega}{2} \zeta \sin \frac{\omega t}{2} \right\} \right] \\
&+ \frac{8}{m \omega \sin \omega t} \int_0^t \int_0^\zeta d\zeta d\sigma f(\zeta) \cdot f(\sigma) \sin \frac{1}{2} \omega(t-\zeta) \sin \frac{\omega}{2} \omega \sin \frac{\omega}{2}(t-\zeta) \sin \frac{1}{2} \omega \zeta \\
&- \frac{2}{m \omega \sin \omega t} \int_0^t \int_0^\zeta d\zeta d\sigma f(\zeta) \cdot f(\sigma) \sin \omega(t-\zeta) \sin \omega \sigma \\
&= \frac{1}{\sin \omega t} \left[\vec{r}_2 \int_0^t f(\zeta) d\zeta \left\{ \sin \omega \zeta - 2 \sin \frac{\omega}{2}(t-\zeta) \sin \frac{\omega}{2} \zeta \sin \frac{\omega t}{2} \right\} \right. \\
&\quad \left. + \vec{r}_1 \int_0^t f(\zeta) d\zeta \left\{ \sin \omega(t-\zeta) - 2 \sin \frac{\omega}{2}(t-\zeta) \sin \frac{\omega}{2} \zeta \sin \frac{\omega t}{2} \right\} \right] \\
&- \frac{2}{m \omega \sin \omega t} \int_0^t \int_0^\zeta d\zeta d\sigma f(\zeta) \cdot f(\sigma) \left\{ \sin \omega(t-\zeta) \sin \omega \sigma \right. \\
&\quad \left. - 4 \sin \frac{1}{2} \omega(t-\zeta) \sin \frac{\omega}{2} \zeta \sin \frac{\omega}{2}(t-\sigma) \sin \frac{1}{2} \omega \sigma \right\} \quad 4.4.22
\end{aligned}$$

From (4.4.13) the classical action can be written as

$$S'_c = \frac{m}{2} \int_0^t \dot{\vec{r}}_c^2(\zeta) d\zeta - \frac{m\omega^2}{4t} \int_0^t d\zeta \int_0^t d\sigma |\vec{r}_c(\zeta) - \vec{r}_c(\sigma)|^2 + \int_0^t f(\zeta) \cdot \vec{r}_c(\zeta) d\zeta$$

one integrates by part the first term of the right to get

$$\begin{aligned}
S'_c &= \frac{m}{2} \left\{ \vec{r}_c(\zeta) \dot{\vec{r}}_c(\zeta) \Big|_0^t - \int_0^t \ddot{\vec{r}}_c(\zeta) \cdot \vec{r}_c(\zeta) d\zeta - \frac{\omega^2}{2t} \int_0^t \int_0^t d\zeta d\sigma |\vec{r}_c(\zeta) - \vec{r}_c(\sigma)|^2 \right\} \\
&\quad + \int_0^t d\zeta f(\zeta) \cdot \vec{r}_c(\zeta)
\end{aligned}$$

$$= \frac{m}{2} \left\{ \overset{\circ}{r}_2 \overset{\circ}{r}_2 - \overset{\circ}{r}_1 \overset{\circ}{r}_1 - \int_0^t \overset{\circ}{r}_c(\zeta) \overset{\circ}{r}_c(\zeta) d\zeta - \frac{\omega^2}{2t} \int_0^t \int_0^t d\zeta d\sigma |\overset{\circ}{r}_c(\zeta) - \overset{\circ}{r}_c(\sigma)|^2 \right\} \\ + \int_0^t d\zeta f(\zeta) \cdot \overset{\circ}{r}_c(\zeta)$$

Multiplying (4.4.14) by $\int_0^t \overset{\circ}{r}_c(\zeta) d\zeta$, one obtains

$$\int_0^t \overset{\circ}{r}_c(\zeta) \overset{\circ}{r}_c(\zeta) d\zeta = -\frac{\omega^2}{2t} \int_0^t \int_0^t d\zeta d\sigma (\overset{\circ}{r}_c(\zeta) - \overset{\circ}{r}_c(\sigma)) \overset{\circ}{r}_c(\zeta) + \int_0^t d\zeta \frac{f(\zeta)}{m} \cdot \overset{\circ}{r}_c(\zeta) \\ \int_0^t \overset{\circ}{r}_c(\zeta) \overset{\circ}{r}_c(\zeta) d\zeta = -\frac{\omega^2}{2t} \int_0^t \int_0^t d\zeta d\sigma (\overset{\circ}{r}_c(\zeta) - \overset{\circ}{r}_c(\sigma)) \overset{\circ}{r}_c(\zeta) - \frac{\omega^2}{2t} \int_0^t \int_0^t d\zeta d\sigma (\overset{\circ}{r}_c(\sigma) - \overset{\circ}{r}_c(\zeta)) \overset{\circ}{r}_c(\zeta) \\ + \int_0^t d\zeta \frac{f(\zeta)}{m} \cdot \overset{\circ}{r}_c(\zeta) \\ = -\frac{\omega^2}{2t} \int_0^t \int_0^t d\zeta d\sigma |\overset{\circ}{r}_c(\zeta) - \overset{\circ}{r}_c(\sigma)|^2 + \int_0^t d\zeta \frac{f(\zeta)}{m} \cdot \overset{\circ}{r}_c(\zeta)$$

This can be substituted into the former equation to get

$$S_c = \frac{m}{2} (\overset{\circ}{r}_2 \overset{\circ}{r}_2 - \overset{\circ}{r}_1 \overset{\circ}{r}_1) + \frac{1}{2} \int_0^t d\zeta f(\zeta) \cdot \overset{\circ}{r}_c(\zeta) \quad 4.4.23$$

Differentiate (4.4.21) with respect to ζ , we get

$$\begin{aligned} \frac{\overset{\circ}{r}}{c}(\zeta) = & \frac{1}{\sin \omega t} \left[\omega(\vec{r}_2 \cos \omega \zeta - \vec{r}_1 \cos \omega(t-\zeta)) - \right. \\ & \left. - (2\omega \sin \frac{1}{2} \omega(t-\zeta) \cos \frac{1}{2} \omega \zeta - 2\omega \cos \frac{1}{2} \omega(t-\zeta) \sin \frac{1}{2} \omega \zeta) \right] \\ & \left\{ \frac{1}{2}(\vec{r}_2 + \vec{r}_1) \sin \frac{1}{2} \omega t - \frac{1}{m \omega} \int_0^t d\sigma f(\sigma) \sin \frac{1}{2} \omega \sigma \sin \frac{1}{2} \omega(t-\sigma) \right\} \\ & + \frac{1}{m} \int_0^t d\sigma f(\sigma) \frac{dg}{d\zeta}(\zeta, \sigma) \end{aligned}$$

$$\begin{aligned} \frac{\overset{\circ}{r}}{c}(\zeta) = & \frac{\omega}{\sin \omega t} \left[\vec{r}_2 \cos \omega \zeta - \vec{r}_1 \cos \omega(t-\zeta) - 2 \sin \omega \left(\frac{t}{2} - \zeta \right) \left\{ \frac{(\vec{r}_2 + \vec{r}_1)}{2} \right\} \sin \frac{1}{2} \omega t - \right. \\ & \left. - \frac{1}{m \omega} \int_0^t d\sigma f(\sigma) \sin \frac{1}{2} \omega \sigma \sin \frac{1}{2} \omega(t-\sigma) \right] + \frac{1}{m} \int_0^t d\sigma f(\sigma) \frac{dg}{d\zeta}(\zeta, \sigma) \quad 4.4.24 \end{aligned}$$

Replacing $\zeta = t$ in (4.4.24), we have

$$\begin{aligned} \frac{\overset{\circ}{r}}{c}(t) = & \frac{\omega}{\sin \omega t} \left[\vec{r}_2 \cos \omega t - \vec{r}_1 + 2 \sin \frac{\omega t}{2} \left\{ \frac{(\vec{r}_2 + \vec{r}_1)}{2} \right\} \sin \frac{\omega t}{2} - \right. \\ & \left. - \frac{1}{m \omega} \int_0^t d\sigma f(\sigma) \sin \frac{\omega \sigma}{2} \sin \frac{\omega}{2}(t-\sigma) \right] \\ & + \frac{1}{m} \int_0^t d\sigma f(\sigma) \frac{dg}{d\zeta}(\zeta, \sigma) \Big|_{\zeta=t} \end{aligned}$$

Replacing $\zeta = 0$ in (4.4.24), we get

$$\begin{aligned} \vec{r}_c^e(0) = & \frac{\omega}{\sin \omega t} \left[\vec{r}_2 - \vec{r}_1 \cos \omega t - 2 \sin \frac{\omega t}{2} \left\{ \frac{(\vec{r}_2 + \vec{r}_1) \sin \omega t}{2} \right. \right. \\ & \left. \left. - \frac{1}{m \omega} \int_0^t d\sigma f(\sigma) \sin \frac{\omega \sigma}{2} \sin \frac{\omega(t-\sigma)}{2} \right\} \right] \\ & + \frac{1}{m} \int_0^t d\sigma f(\sigma) \left. \frac{dg(\zeta, \sigma)}{d\zeta} \right|_{\zeta=0} \end{aligned}$$

$$\begin{aligned} \vec{r}_c^e(t) = & \frac{\omega}{\sin \omega t} \left[\vec{r}_2 \cos \omega t - \vec{r}_1 + \sin^2 \frac{\omega t}{2} (\vec{r}_2 + \vec{r}_1) - \right. \\ & \left. - \frac{2}{m \omega} \sin \frac{\omega t}{2} \int_0^t d\sigma f(\sigma) \sin \frac{\omega \sigma}{2} \sin \frac{\omega(t-\sigma)}{2} \right] \\ & + \frac{1}{m} \int_0^t d\sigma f(\sigma) \left. \frac{dg(\zeta, \sigma)}{d\zeta} \right|_{\zeta=t} \end{aligned} \quad 4.4.25$$

$$\begin{aligned} \vec{r}_c^e(0) = & \frac{\omega}{\sin \omega t} \left[\vec{r}_2 - \vec{r}_1 \cos \omega t - \sin^2 \frac{\omega t}{2} (\vec{r}_2 + \vec{r}_1) \right. \\ & \left. + \frac{2}{m \omega} \sin \frac{\omega t}{2} \int_0^t d\sigma f(\sigma) \sin \frac{\omega \sigma}{2} \sin \frac{\omega(t-\sigma)}{2} \right] \\ & + \frac{1}{m} \int_0^t d\sigma f(\sigma) \left. \frac{dg(\zeta, \sigma)}{d\zeta} \right|_{\zeta=0} \end{aligned} \quad 4.4.26$$

To differentiate (4.4.16) with respect to ζ , we get

$$\frac{dg(\zeta, \sigma)}{d\zeta} = \frac{-1}{\omega \sin \omega t} \left[\omega \sin \omega (t - \sigma) \cos \omega \zeta H(\sigma - \zeta) - \omega \sin \omega \sigma \cos \omega (t - \zeta) H(\zeta - \sigma) \right. \\ \left. - \sin \omega (t - \sigma) \sin \omega \zeta \delta(\sigma - \zeta) + \sin \omega \sigma \sin \omega (t - \zeta) \delta(\zeta - \sigma) \right]$$

Since

$$\left. \frac{dg(\zeta, \sigma)}{d\zeta} \right|_{\zeta=t} = \frac{\sin \omega \sigma}{\sin \omega t}$$

$$\left. \frac{dg(\zeta, \sigma)}{d\zeta} \right|_{\zeta=0} = \frac{-\sin \omega (t - \sigma)}{\sin \omega t}$$

we get

$$\begin{aligned} \overset{\circ}{r}_c(t) &= \frac{\omega}{\sin \omega t} \left(\vec{r}_2 \cos \omega t - \vec{r}_1 + \sin^2 \frac{\omega t}{2} (\vec{r}_2 + \vec{r}_1) \right) \\ &\quad - \frac{2}{m} \cdot \frac{\sin \frac{\omega t}{2}}{\sin \omega t} \int_0^t d\sigma f(\sigma) \sin \frac{\omega \sigma}{2} \sin \frac{\omega}{2} (t - \sigma) \\ &\quad + \frac{1}{m} \int_0^t d\sigma f(\sigma) \frac{\sin \omega \sigma}{\sin \omega t} \end{aligned}$$

$$\begin{aligned} \overset{\circ}{r}_c(t) &= \frac{\omega}{\sin \omega t} \left[\vec{r}_2 \cos \omega t - \vec{r}_1 + \sin^2 \frac{\omega t}{2} (\vec{r}_2 + \vec{r}_1) \right] + \frac{1}{m \sin \omega t} \int_0^t d\sigma f(\sigma) \left((\sin \omega \sigma \right. \\ &\quad \left. - 2 \sin \frac{\omega \sigma}{2} \sin \frac{\omega}{2} (t - \sigma) \sin \frac{\omega t}{2} \right) \end{aligned}$$

One can change the variable σ to ζ , to get

$$\begin{aligned} \dot{\vec{r}}_c(t) = & \frac{\omega}{\sin\omega t} \left[r_2 \cos\omega t - r_1 + (r_2 + r_1) \sin^2 \frac{\omega t}{2} \right] + \frac{1}{m\omega \sin\omega t} \int_0^t d\zeta f(\zeta) \left[\sin\omega\zeta \right. \\ & \left. - 2\sin \frac{\omega\zeta}{2} \sin \frac{\omega}{2} (t-\zeta) \sin \frac{\omega t}{2} \right] \end{aligned} \quad 4.4.27$$

Similarly one obtains

$$\begin{aligned} \dot{\vec{r}}_c(0) = & \frac{\omega}{\sin\omega t} \left[r_2 - r_1 \cos\omega t - (r_2 + r_1) \sin^2 \frac{\omega t}{2} \right] - \frac{1}{m \sin\omega t} \int_0^t d\zeta f(\zeta) \sin\omega(t-\zeta) \\ & - 2\sin \frac{1}{2} \omega t \sin \frac{1}{2} \omega(t-\zeta) \sin \frac{1}{2} \omega\zeta \end{aligned} \quad 4.4.28$$

Then

$$\begin{aligned} \frac{m}{2} (\dot{r}_2 \dot{\vec{r}}_c(t) - \dot{r}_1 \dot{\vec{r}}_c(0)) = & \frac{m\omega}{2\sin\omega t} \left[r_2^2 \cos\omega t - r_1 r_2 + (r_2^2 + r_1 r_2) \sin^2 \frac{\omega t}{2} - r_2 r_1 + r_1^2 \cos\omega t \right. \\ & \left. + (r_2 r_1 + r_1^2) \sin^2 \frac{\omega t}{2} \right] \\ & + \frac{1}{2m\sin\omega t} \left[r_2 \int_0^t d\zeta f(\zeta) \left(\sin\omega\zeta - 2\sin \frac{\omega\zeta}{2} \sin \frac{\omega}{2} (t-\zeta) \sin \frac{\omega t}{2} \right) \right. \\ & \left. + r_1 \int_0^t d\zeta f(\zeta) \left(\sin\omega(t-\zeta) - 2\sin \frac{1}{2} \omega t \sin \frac{1}{2} \omega(t-\zeta) \sin \frac{\omega\zeta}{2} \right) \right] \\ = & \frac{m\omega}{4} \cot \frac{\omega t}{2} |r_2 - r_1|^2 \\ & + \frac{1}{2m \sin\omega t} \left[r_2 \int_0^t d\zeta f(\zeta) \left(\sin\omega\zeta - 2\sin \frac{\omega\zeta}{2} \sin \frac{\omega}{2} (t-\zeta) \sin \frac{\omega t}{2} \right) \right. \\ & \left. + r_1 \int_0^t d\zeta f(\zeta) \left(\sin\omega(t-\zeta) - 2\sin \frac{1}{2} \omega t \sin \frac{1}{2} \omega(t-\zeta) \sin \frac{\omega\zeta}{2} \right) \right] \end{aligned} \quad 4.4.29$$

Substituting (4.4.29) and (4.4.22) into (4.4.23), one obtains

$$\begin{aligned}
 S'_c &= \frac{m\omega}{4} \cot \frac{1}{4} \omega t |\vec{r}_2 - \vec{r}_1|^2 \\
 &+ \frac{m\omega}{2\sin\omega t} \left[\frac{2\vec{r}_2}{m\omega} \cdot \int_0^t d\zeta f(\zeta) (\sin\omega\zeta - 2\sin\frac{1}{2}\omega t \sin\frac{1}{2}\omega(t-\zeta) \sin\frac{1}{2}\omega\zeta) \right. \\
 &+ \frac{2\vec{r}_1}{m\omega} \cdot \int_0^t d\zeta f(\zeta) (\sin\omega(t-\zeta) - 2\sin\frac{1}{2}\omega t \sin\frac{1}{2}\omega(t-\zeta) \sin\frac{1}{2}\omega\zeta) \\
 &- \frac{2}{m^2\omega^2} \int_0^t \int_0^\zeta d\sigma d\sigma f(\zeta) \cdot f(\sigma) (\sin\omega(t-\zeta) \sin\omega\sigma \\
 &\left. - 4 \sin\frac{1}{2}\omega(t-\zeta) \sin\frac{1}{2}\omega\zeta \sin\frac{1}{2}\omega(t-\sigma) \sin\frac{1}{2}\omega\sigma) \right] \quad 4.4.30
 \end{aligned}$$

Setting $f = 0$, one obtains

$$S_{0,c} = \frac{m}{4} \omega \cot \frac{\omega t}{2} |\vec{r}_2 - \vec{r}_1|^2 \quad 4.4.31$$

The Evaluation of $\langle \vec{r}(\zeta) - \vec{r}(\sigma) \rangle_{S_0}$ and $\langle (\vec{r}_\zeta - \vec{r}_\sigma)^2 \rangle_{S_0}$ proceeds as

follows :

From (4.4.10) we have

$$\langle \vec{r}_\zeta \rangle_{S_0} = \frac{\delta S_c}{\delta \vec{r}_\zeta} \Big|_{f=0}$$

Thus by differentiating eq. (4.4.10) with respect to $f(\zeta)$ and setting $f = 0$, we get

$$\langle \vec{r}(\zeta) \rangle_{S_0} = \frac{m\omega}{2\sin\omega t} \left\{ \frac{2\vec{r}_2}{m\omega} (\sin\omega\zeta - 2\sin\frac{\omega t}{2} \sin\frac{\omega}{2}(t-\zeta) \sin\frac{\omega\zeta}{2}) \right. \\ \left. + \frac{2\vec{r}_1}{m\omega} (\sin\omega(t-\zeta) - 2\sin\frac{\omega}{2} t \sin\frac{\omega}{2}(t-\zeta) \sin\frac{\omega\zeta}{2}) \right\}$$

$$\text{Similarly } \langle \vec{r}_\sigma \rangle_{S_0} = \frac{m\omega}{2\sin\omega t} \left\{ \frac{2\vec{r}_2}{m\omega} (\sin\omega\sigma - 2\sin\frac{\omega t}{2} \sin\frac{\omega}{2}(t-\sigma) \sin\frac{\omega\sigma}{2}) \right. \\ \left. + \frac{2\vec{r}_1}{m\omega} (\sin\omega(t-\sigma) - 2\sin\frac{\omega}{2} t \sin\frac{\omega}{2}(t-\sigma) \sin\frac{\omega\sigma}{2}) \right\}$$

$$\langle \vec{r}_\zeta - \vec{r}_\sigma \rangle_{S_0} = \langle \vec{r}_\zeta \rangle_{S_0} - \langle \vec{r}_\sigma \rangle_{S_0} \\ = \frac{m\omega}{2\sin\omega t} \left\{ \frac{2\vec{r}_2}{m\omega} (\sin\omega\zeta - 2\sin\frac{\omega t}{2} \sin\frac{\omega}{2}(t-\zeta) \sin\frac{\omega\zeta}{2} - \sin\omega\sigma \right. \\ \left. + 2\sin\frac{\omega t}{2} \sin\frac{\omega}{2}(t-\sigma) \sin\frac{\omega\sigma}{2}) \right. \\ \left. - \frac{2\vec{r}_1}{m\omega} (\sin\omega(t-\sigma) - \sin\omega(t-\zeta) - 2\sin\frac{\omega}{2} t \sin\frac{\omega}{2}(t-\sigma) \sin\frac{\omega\sigma}{2} \right. \\ \left. + 2\sin\frac{\omega t}{2} \sin\frac{\omega}{2}(t-\zeta) \sin\frac{\omega\zeta}{2}) \right\} \\ = \vec{r}_2 \left\{ \frac{\sin\omega\zeta - \sin\omega\sigma}{\sin\omega t} - \frac{1}{\sin\omega t} \left(2\sin\frac{\omega t}{2} \sin\frac{\omega}{2}(t-\zeta) \sin\frac{\omega\zeta}{2} \right. \right. \\ \left. \left. - 2\sin\frac{\omega t}{2} \sin\frac{\omega}{2}(t-\sigma) \sin\frac{\omega\sigma}{2} \right) \right\} + \vec{r}_1 \left\{ \frac{\sin\omega(t-\zeta) + \sin\omega(t-\sigma)}{\sin t} \right. \\ \left. + \frac{1}{\sin\omega t} \left(2\sin\frac{\omega t}{2} \sin\frac{\omega}{2}(t-\sigma) \sin\frac{\omega\sigma}{2} - 2\sin\frac{\omega t}{2} \sin\frac{\omega}{2}(t-\zeta) \sin\frac{\omega\zeta}{2} \right) \right\}$$

By using the identity

$$\frac{\sin\omega\zeta - \sin\omega\sigma}{\sin\omega t} = \sin\frac{\omega}{2}(\zeta - \sigma) \cos\frac{\omega}{2}(t - (\zeta + \sigma)) / \sin\frac{\omega t}{2}$$

and $\frac{\sin\omega(t - \zeta) - \sin\omega(t - \sigma)}{\sin\omega t} = \frac{-\sin\omega(\zeta - \sigma) \cos\frac{\omega}{2}(t - (\zeta + \sigma))}{\sin\frac{\omega t}{2}}$, we get

$$\langle \vec{r}_\zeta - \vec{r}_\sigma \rangle_{S_0} = \left\{ \sin\frac{\omega}{2}(\zeta - \sigma) \cos\frac{\omega}{2}(t - (\zeta + \sigma)) / \sin\frac{\omega t}{2} \right\} \cdot (\vec{r}_2 - \vec{r}_1) \quad 4.4.33$$

From (4.4.12)

$$\langle \vec{r}_\zeta \vec{r}_\sigma \rangle_{S_0} = \left\{ \frac{\hbar}{i} \frac{\delta^2 S_{cl}}{\delta f_\zeta \delta f_\sigma} + \frac{\delta S_{cl}}{\delta f_\zeta} \cdot \frac{\delta S_{cl}}{\delta f_\sigma} \right\} \Big|_{f=0}$$

Thus one can obtain $\langle \vec{r}_\zeta \vec{r}_\sigma \rangle_{S_0}$ by differentiating (4.4.30). We get

$$\begin{aligned} \langle \vec{r}_\zeta \vec{r}_\sigma \rangle_{S_0} = & -3 \cdot \frac{1\hbar}{2i} \frac{m\omega}{2\sin\omega t} \left\{ \frac{2}{m^2\omega^2} (\sin\omega(t - \zeta)\sin\omega\sigma - 4\sin\frac{\omega}{2}(t - \zeta)\sin\frac{\omega}{2}\sin\frac{\omega}{2}(t - \sigma)) \right. \\ & + \left(\frac{m\omega}{2\sin\omega t} \right)^2 \left\{ \frac{2r_2}{m\omega} (\sin\omega\zeta - 2\sin\omega t \sin\frac{\omega}{2}(t - \zeta)\sin\frac{\omega}{2}\zeta) + \frac{2r_1}{m\omega} (\sin\omega(t - \zeta) \right. \\ & \left. \left. - 2\sin\omega t \sin\frac{\omega}{2}(t - \zeta)\sin\frac{\omega}{2}\zeta) \right\} \left\{ \frac{2r_2}{m\omega} (\sin\omega\zeta - 2\sin\frac{\omega}{2}t \right. \right. \\ & \left. \left. \sin\frac{\omega}{2}(t - \sigma)\sin\frac{\omega}{2}\sigma) + \frac{2r_1}{m\omega} (\sin\omega(t - \sigma) - 2\sin\omega t \sin\frac{\omega}{2}(t - \sigma)\sin\frac{\omega}{2}\sigma) \right\} \right\} \end{aligned}$$

4.4.34

Since in three dimensions, $\nabla f = 3$, and $\frac{1}{2}$ arises from symmetry of S_{cl}

we get

$$\langle r_{\zeta}^2 \rangle_{S_0} = \left\{ \frac{\hbar}{i} \frac{\delta^2 S'}{\delta f_{\zeta} \delta f_{\sigma}} \Big|_{\sigma=\zeta} + \frac{\delta^2 S'}{\delta f_{\zeta}} \cdot \frac{\delta S'}{\delta f_{\sigma}} \Big|_{\sigma=\zeta} \right\} \Big|_{f=0} \quad 4.4.35$$

$$\langle r_{\sigma}^2 \rangle_{S_0} = \left\{ \frac{\hbar}{i} \frac{\delta^2 S'}{\delta f_{\zeta} f_{\sigma}} \Big|_{\zeta=\sigma} + \frac{\delta^2 S'}{\delta f_{\zeta}} \cdot \frac{\delta S'}{\delta f_{\sigma}} \Big|_{\zeta=\sigma} \right\} \Big|_{f=0} \quad 4.4.36$$

$$\langle (\vec{r}_{\zeta} - \vec{r}_{\sigma})^2 \rangle = \langle r_{\zeta}^2 \rangle_{S_0} - 2\langle \vec{r}_{\zeta} \vec{r}_{\sigma} \rangle_{S_0} + \langle r_{\sigma}^2 \rangle_{S_0} \quad 4.4.37$$

By using (4.4.34) to (4.4.37) one gets

$$\begin{aligned} \langle (\vec{r}_{\zeta} - \vec{r}_{\sigma})^2 \rangle &= \frac{-3\hbar}{2i} \frac{m\omega}{2\sin\omega t} \left\{ \frac{2}{m^2\omega^2} (\sin\omega(t-\zeta)\sin\omega\zeta - 2\sin\omega(t-\zeta)\sin\omega\sigma \right. \\ &\quad \left. + \sin\omega(t-\sigma)\sin\omega\sigma) - 4\left(\frac{\sin\omega}{2}(t-\zeta)\frac{\sin\omega\zeta}{2} - \frac{\sin\omega}{2}(t-\sigma)\frac{\sin\omega\sigma}{2}\right)^2 \right\} \\ &\quad + \left\{ \vec{r}_2 \left[\frac{\sin\omega\zeta}{\sin\omega t} - \frac{\sin\omega}{2}(t-\zeta)\frac{\sin\omega\zeta}{\cos\omega t} \right] \right. \\ &\quad \left. - \frac{(\sin\omega - \frac{\sin\omega}{2}(t-\sigma)\frac{\sin\omega\sigma}{\cos\omega t})}{\sin\omega t} \right\} \\ &\quad + \vec{r}_1 \left[\frac{(\sin\omega(t-\zeta) - \frac{\sin\omega(t-\zeta)\sin\omega\zeta}{\cos\omega t})}{\sin\omega t} \right. \\ &\quad \left. - \frac{(\sin\omega(t-\sigma) - \frac{\sin\omega(t-\sigma)\sin\omega\sigma}{\cos\omega t})}{\sin\omega t} \right] \Big\}^2 \quad 4.4.38 \end{aligned}$$

And using the identity

$$\begin{aligned}
& (\sin\omega(t-\zeta)\sin\omega\zeta - 2\sin\omega(t-\zeta)\sin\omega\sigma + \sin\omega(t-\sigma)\sin\omega\sigma) - \\
& - 4\left(\frac{\sin\omega(t-\zeta)\sin\omega\zeta}{2} - \frac{\sin\omega(t-\sigma)\sin\omega\sigma}{2}\right)^2 \\
& = 4\frac{\sin\omega(\zeta-\sigma)\sin\omega(t-(\zeta-\sigma))\cos\omega t}{2}
\end{aligned}$$

(4.4.38) becomes

$$\begin{aligned}
\langle (\vec{r}_\zeta - \vec{r}_\sigma)^2 \rangle &= \frac{3}{2} \frac{i\hbar}{m\omega} \cdot \frac{4 \sin\omega(\zeta-\sigma)\sin\omega(t-(\zeta-\sigma))}{\sin\frac{\omega t}{2}} \\
&+ \left\{ \frac{\sin\omega(\zeta-\sigma)\cos\omega(t-(\zeta+\sigma))}{\sin\frac{\omega t}{2}} \right\}^2 (\vec{r}_2 - \vec{r}_1)^2
\end{aligned} \tag{4.4.39}$$

Substituting (4.4.38) and (4.4.39) into (4.4.6), one has

$$\begin{aligned}
\langle \exp(i\vec{k} \cdot (\vec{r}_\zeta - \vec{r}_\sigma)) \rangle_{S_0} &= \exp \left[\frac{i\vec{k} \cdot (\sin\omega(\zeta-\sigma)\cos\omega(t-(\zeta+\sigma))) (\vec{r}_2 - \vec{r}_1)}{\sin\frac{\omega t}{2}} \right. \\
&+ \frac{i^2 k^2}{2} \left\{ \frac{1}{3} \cdot \frac{3}{2} \frac{i\hbar}{m\omega} \cdot \frac{4\sin\omega(\zeta-\sigma)\sin\omega(t-(\zeta-\sigma))}{\sin\frac{\omega t}{2}} \right. \\
&+ \frac{1}{3} \left(\frac{\sin\omega(\zeta-\sigma)\cos\omega(t-(\zeta+\sigma))}{\sin\frac{\omega t}{2}} \right)^2 (\vec{r}_2 - \vec{r}_1)^2 - \frac{1}{3} \frac{(\sin\omega(\zeta-\sigma)\cos\omega(t-(\zeta+\sigma))) (\vec{r}_2 - \vec{r}_1)^2}{\sin\frac{\omega t}{2}} \left. \left. \right\} \right] \\
&= \exp \left\{ \frac{i\vec{k} \cdot (\sin\omega(\zeta-\sigma)\cos\omega(t-(\zeta+\sigma))) (\vec{r}_2 - \vec{r}_1)}{\sin\frac{\omega t}{2}} + \frac{i^2 k^2}{2} \cdot \frac{2i\hbar \sin\omega(\zeta-\sigma)\sin\omega(t-(\zeta-\sigma))}{m\omega \sin\frac{\omega t}{2}} \right\}
\end{aligned} \tag{4.4.40}$$

Going further, we get

$$\begin{aligned} \frac{m\omega^2}{4} \int_0^t \int_0^t d\zeta d\sigma \langle (\vec{r}_\zeta - \vec{r}_\sigma)^2 \rangle &= \frac{m\omega^2}{2} \int_0^t \int_0^t d\zeta d\sigma \nabla_{\vec{k}}^2 \langle \exp i\vec{k} \cdot (\vec{r}_\zeta - \vec{r}_\sigma) \rangle \Big|_{\vec{k}=0} \\ &= \frac{3}{2} i\hbar \left(\frac{\omega}{2} t \cot \frac{\omega t}{2} - 1 \right) \\ &\quad + \frac{1}{2} m (\vec{r}_2 - \vec{r}_1)^2 \left[\frac{\omega t}{2} \cot \frac{\omega t}{2} - \left(\frac{1}{2} \frac{\sin \omega t}{2} \right) \right] \quad 4.4.41 \end{aligned}$$

After (4.4.40) and (4.4.41) are substituted into (4.4.4)

we have

$$\begin{aligned} \langle S_0 \rangle_{S_0} &= \frac{i}{2\hbar} \xi \frac{Q}{n\pi} \int_0^t \int_0^t d\zeta d\sigma \int \frac{d^3\vec{k}}{(2\pi)^3} \left(\frac{4\pi}{k^2 + Q^2} \right)^2 \\ &\quad \exp \left\{ \frac{i\vec{k} \cdot (\sin \frac{\omega}{2} (\zeta - \sigma) \cos \frac{\omega}{2} (t - (\zeta + \sigma)) (\vec{r}_2 - \vec{r}_1)}{\sin \frac{\omega t}{2}} \right. \\ &\quad \left. + i^2 k^2 \left(\frac{i\hbar}{m\omega} \frac{\sin \frac{\omega}{2} (\zeta - \sigma) \sin \frac{\omega}{2} (t - (\zeta + \sigma))}{\sin \frac{\omega t}{2}} \right) - \frac{3}{2} i\hbar \left(\frac{\omega}{2} t \cot \frac{\omega t}{2} - 1 \right) \right\} \quad 4.4.42 \end{aligned}$$

$$\text{Since } G(\vec{r}_2, \vec{r}_1; t) = \exp \left\{ \frac{i}{\hbar} \langle S - S_0 \rangle_{S_0} \right\} G_0(\vec{r}_2, \vec{r}_1; t) \quad 4.4.43$$

we get after (4.4.3) and (4.4.42) are substituted into (4.4.43)

$$\begin{aligned}
G(\mathbf{r}_2, \mathbf{r}_1; t) = & \left(\frac{m}{2\pi i \hbar t} \right)^{3/2} \left(\frac{\omega t}{2 \sin \frac{\omega t}{2}} \right) \exp \left\{ \frac{3}{2} \left(\frac{\omega t \cot \omega t}{2} - 1 \right) \frac{-i}{\hbar} E_0 t \right. \\
& - \frac{\xi}{n} \frac{Q}{2\pi} \int \frac{d^3 \vec{k}}{(2\pi)^3} \left(\frac{4\pi}{k^2 + Q^2} \right)^2 \int_0^t \int_0^\zeta d\zeta d\sigma \exp(i\mathbf{k} \cdot (\vec{\mathbf{r}}_2 - \vec{\mathbf{r}}_1) \sin \frac{\omega(\zeta - \sigma)}{2}) \\
& \left. \frac{\cos \frac{\omega(t - (\zeta + \sigma))}{2} - ik^2 \frac{\hbar}{m\omega} \frac{\sin \frac{\omega(\zeta - \sigma)}{2} \sin \frac{\omega(t - (\zeta - \sigma))}{2}}{\sin \frac{\omega t}{2}} \right) \\
& - \frac{im}{2\hbar} \left(\frac{\omega t \cot \omega t}{2} + \left(\frac{1}{2} \omega t \operatorname{cosec} \frac{\omega t}{2} \right)^2 \right) \left(\frac{\vec{\mathbf{r}}_2 - \vec{\mathbf{r}}_1}{2t} \right) \left. \right\} \quad 4.4.44
\end{aligned}$$

Inserting the identity

$$(k^2 + Q^2)^{-2} = \int_0^\infty dy \exp \left\{ -(k^2 + Q^2)y \right\}$$

into the second term of right hand members of (4.4.44); it becomes

$$\begin{aligned}
(4\pi)^2 \int_0^t \int_0^\zeta d\zeta d\sigma \int_0^\zeta \frac{d\vec{k}}{(2\pi)^3} \int_0^\infty dy \exp(-(k^2 + Q^2)y) \\
- \frac{ik^2 \hbar}{m\omega} \frac{\sin \frac{\omega(\zeta - \sigma)}{2} \sin \frac{\omega(t - (\zeta - \sigma))}{2}}{\sin \frac{\omega t}{2}} \\
+ \frac{i\mathbf{k} \cdot (\vec{\mathbf{r}}_2 - \vec{\mathbf{r}}_1) \sin \frac{\omega(\zeta - \sigma)}{2} \cos \frac{\omega(t - (\zeta + \sigma))}{2}}{\sin \frac{\omega t}{2}} \left. \right)
\end{aligned}$$

If we write

$$y + \frac{i\hbar}{m\omega} \cdot \frac{\sin \frac{\omega(\zeta - \sigma)}{2} \sin \frac{\omega(t - (\zeta - \sigma))}{2}}{\sin \frac{\omega t}{2}} = A(\zeta - \sigma, y)$$

and

$$\frac{(\vec{r}_2 - \vec{r}_1) \sin \omega(\zeta - \sigma) \cos \omega(t - (\zeta + \sigma))}{\sin \frac{\omega t}{2}} = B(\zeta, \sigma)$$

$$= \int_0^t \int_0^\zeta d\zeta d\sigma \frac{1}{(2\pi)^3} \int_0^\infty dy y e^{-Q^2 y} \int d\vec{k} e^{-ik^2 A(\zeta - \sigma, y) + i\vec{k} \cdot B(\zeta, \sigma)}$$

where

$$\int d\vec{k} e^{-ik^2 A + i\vec{k} \cdot B} = 4\pi \int_0^\infty k^2 dk \int_{-1}^1 d\mu e^{-ik^2 A + ik \mu B}$$

we get

$$= \sqrt{4\pi} \int_0^t \int_0^\zeta d\zeta d\sigma \int_0^\infty dy y A^{-3/2}(\zeta - \sigma, y) e^{-Q^2 y - B^2(\zeta, \sigma)/4A(\zeta - \sigma, y)} \quad 4.4.45$$

After substituting (4.4.45) into (4.4.44) and we get

$$G(\vec{r}_2, \vec{r}_1; t) = \left(\frac{m}{2\pi i \hbar t} \right)^{3/2} \left(\frac{\omega t}{2 \sin \omega t} \right)^3 \exp \left\{ \frac{3}{2} \left(\frac{\omega t \cot \omega t}{2} - 1 \right) - \frac{i E_0 t}{\hbar} \right.$$

$$\left. - \frac{1}{\hbar} \frac{\zeta}{2n} \frac{Q}{2\pi} \int_0^t \int_0^t d\zeta d\sigma \int_0^\infty dy y A(\zeta - \sigma, y)^{-3/2} \right.$$

$$\left. \cdot \exp(-Q^2 y - B^2(\zeta, \sigma)/4A(\zeta - \sigma, y)) \right\}$$

$$- \frac{i m}{2\hbar} \left(\frac{\omega t \cot \omega t}{2} + \left(\frac{1}{2} t \operatorname{cosec} \frac{\omega t}{2} \right)^2 \right) |\vec{r}_2 - \vec{r}_1|^2 / 2t \quad 4.4.46$$

Because of the property of translational invariance of average Green's function, one has

$$G(\vec{r}_2, \vec{r}_1; t) = G(\vec{r}_2 - \vec{r}_1; t) \quad 4.4.47$$

Setting $\vec{r}_1 = \vec{r}_2$ (4.4.46) becomes

$$G(0,0;t) = \left(\frac{m}{2\pi i \hbar t}\right)^{3/2} \left(\frac{\omega t}{2 \sin \frac{\omega t}{2}}\right)^3 \exp \left\{ \frac{3}{2} \left(\frac{\omega t}{2} \cot \frac{\omega t}{2} - 1\right) \frac{-i}{\hbar} E_0 t \right. \\ \left. - \frac{1}{\hbar} \frac{\xi Q}{n 2\pi} \int_0^t \int_0^\zeta d\zeta d\sigma \int_0^\infty dy y \Lambda(\zeta - \sigma, y) \exp(-Q^2 y) \right\} \quad 4.4.48$$

4.5 The Density of States ^{27,30,32,4}

The density of states can be obtained as follows by taking the Fourier transform of $G(\vec{r}_2, \vec{r}_1; t)$

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

and then taking the trace, i.e.,

$$\rho(E) = \frac{1}{2\pi \hbar \Omega} \text{Tr} \int_{-\infty}^{\infty} e^{iEt/\hbar} G(\vec{r}_2, \vec{r}_1; t) dt \quad 4.5.1$$

where Tr denotes the trace $\int dr$

Because of the translational invariance of the system, there is no preferred origin or direction and G has the property

$$G(\vec{r}_2, \vec{r}_1; t) = G(\vec{r}_2 - \vec{r}_1; t) \quad 4.5.2$$

Thus (4.5.1) can be written as

$$\rho(E) = \frac{1}{2\pi\hbar\Omega} \int dr \int_{-\infty}^{\infty} e^{iEt/\hbar} G(\vec{r}\vec{r}; t) dt \quad 4.5.3$$

After substituting (4.2.2.4) into (4.5.3), we obtain.

$$\rho(E) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \oint D(\vec{r}(\zeta)) \exp \left\{ \frac{i}{\hbar} \frac{m}{2} \int_0^t d\zeta \dot{\vec{r}}^2(\zeta) - \frac{i}{\hbar} (E_0 - E)t \right. \\ \left. - \frac{n}{2\hbar^2} \int_0^t d\zeta \int_0^t d\sigma W(\vec{r}(\zeta) - \vec{r}(\sigma)) \right\} \quad 4.5.4$$

where \oint represents $\vec{r}(0) = \vec{r}(t) = \vec{r}$

$$\text{Thus } \rho(E) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt G(0,0,t) \exp\left(\frac{i}{\hbar} Et\right) \quad 4.5.5$$

After one substitutes (4.4.48) into (4.5.5). One obtains

$$\rho(E) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \left(\frac{m}{2\pi i \hbar t} \right)^{3/2} \left(\frac{\omega t}{2 \sin \frac{\omega t}{2}} \right)^3 \exp \left\{ \frac{3}{2} \left(\frac{\omega t \cot \frac{\omega t}{2}}{2} - 1 \right) - \frac{i}{\hbar} (E_0 - E)t \right. \\ \left. - \frac{1}{\hbar^2} \frac{\xi Q}{n} \frac{Q}{2\pi} \int_0^t \int_0^t d\zeta d\sigma \int_0^{\infty} dy y A^{-3/2}(\zeta - \sigma, y) e^{-Q^2 y} \right\} \quad 4.5.6$$

Now noting that

$$\int_0^t d\zeta \int_0^t d\sigma A(\zeta - \sigma, y)^{-3/2} \quad \text{by letting } \zeta - \sigma = x \\ \int_0^t d\zeta \int_0^t dx A(x, y)^{-3/2} = t \int_0^t dx A(x, y)^{-3/2}$$

and

$$\int_0^t d\zeta \int_0^t dx f(x) = \int_0^t d\zeta \int_0^\zeta dx f(x) + \int_0^t d\zeta \int_\zeta^t dx f(x)$$

we get

$$t \int_0^t dx A(x,y)^{-3/2} = \int_0^t d\zeta \int_0^\zeta dx A(x,y)^{-3/2} + \int_0^t d\zeta \int_0^{t-\zeta} dx A(t-x,y)^{-3/2}$$

Since $A(x,y)$ is translational invariant in period t , we have

$$A(t-x,y)^{-3/2} = A(x,y)^{-3/2}$$

Therefore

$$t \int_0^t dx A(x,y)^{-3/2} = \int_0^t d\zeta \int_0^\zeta dx A(x,y)^{-3/2} + \int_0^t d\zeta \int_0^\zeta dx A(x,y)^{-3/2}$$

$$\int_0^t d\zeta \int_0^\zeta dx A(x,y)^{-3/2} = \frac{t}{2} \int_0^t dx A(x,y)^{-3/2} \quad 4.5.7$$

(4.5.7) is substituted into (4.5.6). Thus

$$\rho(E) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \left(\frac{m}{2\pi i\hbar t} \right)^{3/2} \left(\frac{\omega t}{2 \sin \omega t} \right)^3 \exp \left\{ \frac{3}{2} \left(\frac{\omega t \cot \omega t}{2} - 1 \right) - \frac{i}{\hbar} (E_0 - E)t \right. \\ \left. - \frac{1}{\hbar^2} \frac{\xi}{n} \frac{Q}{2\pi} \cdot \frac{t}{2} \int_0^t dx \int_0^\infty dy e^{-Q^2 y} j(x,y)^{-3/2} \right\}$$

where

$$j(x,y) = y + \frac{i\hbar}{m^* \omega} \left(\frac{\sin \omega x}{2} \frac{\sin \omega (t-x)}{2} / \sin \omega t \right) \quad 4.5.8$$

For convenience one transforms the quantity $\rho(E)$ into dimensionless quantity

$$\rho(E) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \left(\frac{m}{2\pi i\hbar t} \right)^{3/2} \left(\frac{\omega t}{2\sin\frac{\omega t}{2}} \right)^3 \exp \left\{ \frac{3}{2} \left(\frac{\omega t}{2} \cot \frac{\omega t}{2} - 1 \right) + \frac{i(E-E_0)t}{\hbar} \right\}$$

$$= \frac{\xi_1}{2\hbar^2} \frac{Qt}{\sqrt{\pi}} \int_0^t dx \int_0^{\infty} dy y e^{-Q^2 y} j(x,y) \quad 4.5.9$$

where $j(x,y) = \left(y + \frac{i\hbar}{m\omega} \frac{\sin\omega x}{2} \frac{\sin\omega(t-x)}{2} / \frac{\sin\omega t}{2} \right)$

Since $E_{\omega} = \hbar\omega$

and $E_Q = \frac{\hbar^2 Q^2}{2m}$

we have

$$\frac{\hbar}{m\omega} = \frac{\hbar^2}{m\hbar\omega} = 2E_Q/E_{\omega}Q^2$$

and so

$$f(y,x,t) = \left\{ y + \frac{2i}{Q^2} \frac{E_Q}{E_{\omega}} \frac{\sin\omega x}{2} \frac{\sin\omega(t-x)}{2} / \frac{\sin\omega t}{2} \right\}^{-3/2}$$

Letting $\frac{y}{Q^2} = y'$ then $dy = \frac{dy'}{Q^2}$

we have

$$e^{-Q^2 y} = e^{-\frac{Q^2 y'}{Q^2}} = e^{-y'}$$

Letting

$$x = tx' \quad \text{then} \quad dx = t dx'$$

we get

$$f(y', x', t) = \left(\frac{y'}{Q^2} + \frac{2i}{Q^2} \frac{E_Q}{E_\omega} \sin \omega t x' \sin \omega(t-x't) / \sin \frac{\omega t}{2} \right)^{-3/2}$$

Letting $t = \frac{2}{\omega} t'$ which gives $dx = t dx'$

we get

$$f(y', x', t) = \left(\frac{y'}{Q^2} + \frac{2i}{Q^2} \frac{E_Q}{E_\omega} \sin \left(\frac{\omega}{2} \cdot \frac{2}{\omega} t' x' \right) \sin \frac{2t'}{\omega} \left(\frac{1-x'}{2} \right) / \sin \frac{\omega}{2} \cdot \frac{2t'}{\omega} \right)^{-3/2}$$

Noticing that

$$j(x', y') = Q^3 \left(y' + \frac{2i}{E_\omega} \frac{E_Q}{E_\omega} \sin t'(1-x') / \sin t' \right)$$

$$\text{and } \left(\frac{m}{2\pi i \hbar t} \right)^{3/2} = \left(\frac{m}{2\pi i \hbar \frac{2t'}{\omega}} \right)^{3/2} = \left(\frac{m\omega}{4\pi i \hbar t'} \right)^{3/2}$$

$$dt = \frac{2dt'}{\omega}$$

$$\frac{\omega t}{2 \sin \frac{\omega t}{2}} = \left(\frac{2t'}{2 \sin t'} \right)^3 = \left(\frac{t'}{\sin t'} \right)^3$$

$$\frac{3}{2} \left(\frac{\omega t \cot \frac{\omega t}{2}}{2} - 1 \right) = \frac{3}{2} (t' \cot t' - 1)$$

$$\frac{i}{\hbar} (E - E_0) t = \frac{2i}{\hbar \omega} (E - E_0) t' = \frac{2i}{E_\omega} (E - E_0) t' = \frac{2i}{E_Q} (E - E_0) t' \cdot \frac{E_Q}{E_\omega}$$

$$\xi \cdot \frac{1}{2\hbar^2} \frac{Qt}{\sqrt{\pi}} = \xi \cdot \frac{1}{2\hbar^2 \sqrt{\pi}} \cdot \frac{2}{\omega} t'^2 = \frac{1}{\hbar} \xi \frac{Q}{\pi} \cdot \frac{t'}{\hbar \omega} = \frac{1}{\hbar} \xi \frac{Q}{\sqrt{\pi}} \frac{t'}{E_\omega}$$

We find that

$$\rho(E) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \frac{2}{\omega} dt \left(\frac{m\omega}{4\pi i \hbar t} \right)^{3/2} \cdot \left(\frac{t}{\sin t} \right)^3 \cdot \exp \left\{ \frac{3}{2} (t \cot t - 1) \frac{-2i(E_0 - E)t \cdot \frac{E_Q}{E_\omega}}{E_Q} \right. \\ \left. - \frac{1}{\hbar} \frac{\xi Q}{\sqrt{\pi}} \cdot \frac{t}{E_\omega} \int_0^1 \frac{2}{\omega} t dx \int_0^\infty \frac{y}{Q^2} \frac{dy}{Q^2} e^{-y} f(y, x, t) \right\}$$

$$\rho(E) = \frac{1}{2\pi\hbar} \cdot \frac{2}{\omega} \left(\frac{m\omega}{4\pi i \hbar} \right)^{3/2} \int_{-\infty}^{\infty} dt \left(\frac{1}{t} \right)^{3/2} \cdot \left(\frac{t}{\sin t} \right)^3 \cdot \exp \left\{ \frac{3}{2} (t \cot t - 1) \frac{-2i(E_0 - E)t \frac{E_Q}{E_\omega}}{E_Q} \right. \\ \left. - \frac{1}{\hbar} \frac{\xi Q}{\sqrt{\pi}} \frac{t^2}{E_\omega} \cdot \frac{2}{\omega} \cdot \frac{1}{Q} \int_0^1 dx \int_0^\infty y dy e^{-y} f(y, x, t) \right\}$$

or

$$\rho(E) = \frac{1}{\pi\hbar \omega} \left(\frac{m\omega}{4\pi\hbar} \right)^{3/2} \int_{-\infty}^{\infty} dt \left(\frac{1}{t} \right)^{3/2} \left(\frac{t}{\sin t} \right)^3 \exp \left\{ \frac{3}{2} (t \cot t - 1) \frac{-2i(E_0 - E)t \cdot \frac{E_Q}{E_\omega}}{E_Q} \right. \\ \left. - \frac{1}{\hbar} \frac{\xi}{\pi} \frac{t^2}{\omega} \int_0^1 dx \int_0^\infty y dy e^{-y} \frac{(y + 2i \frac{E_Q}{E_\omega} \frac{\sin t x \sin t(1-x)})}{\sin t} \right\}^{-3/2}$$

Making the transformation

$$\frac{1}{\pi\hbar \omega} \left(\frac{m\omega}{4\pi\hbar} \right)^{3/2} = \frac{1}{8\pi^2} \pi \cdot \sqrt{\frac{m\omega}{\hbar}} \cdot \frac{m}{\hbar^2} = \frac{1}{8\pi^2 \sqrt{\pi}} \cdot \sqrt{\frac{m\omega}{\hbar}} Q^2 \cdot \frac{2}{2} \frac{m}{\hbar^2 Q^2} \\ = \frac{1}{16\pi^2 \sqrt{\pi}} \cdot \sqrt{\frac{m\omega}{\hbar}} Q^2 \cdot \frac{1}{E_Q} = \frac{1}{16\pi^2 \sqrt{\pi}} \cdot \frac{Q^2}{E_Q} \sqrt{\frac{\hbar \cdot m\omega}{\hbar^2}} \\ = \frac{1}{16\pi^2 \sqrt{\pi}} \cdot \frac{Q^2}{E_Q} \cdot Q \sqrt{\frac{\hbar \cdot \omega}{\hbar^2 Q^2}} \cdot \frac{1}{\sqrt{2}} \\ = \frac{1}{16\pi^2 \sqrt{\pi}} \frac{Q^3}{E_Q} \cdot \sqrt{\frac{E_\omega}{2E_Q}}$$

and

$$\frac{1}{\hbar} \frac{\xi}{\sqrt{\pi}} \cdot \frac{1}{E_{\omega}} \cdot \frac{2}{\omega} = \frac{2}{\sqrt{\pi}} \frac{\xi}{E_{\omega}^2} = \frac{2}{\sqrt{\pi}} \frac{\xi}{E_Q^2} \cdot \frac{E_Q^2}{E_{\omega}^2} = \frac{1}{2\sqrt{\pi}} \frac{\xi}{E_Q^2} \cdot \frac{4E_Q^2}{E_{\omega}^2}$$

letting

$$\frac{2E_Q}{E_{\omega}} = z^2 \quad \text{and} \quad \xi' = \xi/E_Q^2$$

$$\frac{1}{\pi \hbar \omega} \left(\frac{m\omega}{4\pi \hbar} \right)^{3/2} = \frac{1}{16\pi^2 \sqrt{\pi}} \frac{E_Q^3}{E_{\omega}^3} \cdot \sqrt{\frac{E_{\omega}}{2E_Q}} = \frac{1}{16\pi^2 \sqrt{\pi}} \frac{E_Q^3}{E_{\omega}^3} \cdot \frac{1}{z}$$

$$\frac{1}{\hbar \sqrt{\pi}} \frac{2}{\omega} \cdot \frac{1}{E_{\omega}} = \frac{1}{2\sqrt{\pi}} \frac{\xi}{E_Q^2} \cdot \frac{4E_Q^2}{E_{\omega}^2} = \frac{1}{2\sqrt{\pi}} \xi z^4$$

$$\frac{E_0 - E}{E_Q} = v$$

$$\frac{2i(E_0 - E)}{E_Q} \cdot \frac{E_Q}{E_{\omega}} = \frac{i(E_0 - E)}{E_Q} \cdot \frac{2E_Q}{E_{\omega}} = ivz^2$$

We get

$$\rho(E) = \frac{1}{16\pi^2 \sqrt{\pi}} \frac{E_Q^3}{E_{\omega}^3} \cdot \frac{1}{z} \int_{-\infty}^{\infty} dt (it)^{-3/2} \left(\frac{1}{\sin t} \right)^3 \exp\left\{ \frac{3}{2}(t \cot t - 1) \right. \\ \left. - ivz^2 t \right.$$

$$\left. - \frac{1}{2\sqrt{\pi}} \xi z^4 t^2 \int_0^1 dx \int_0^{\infty} dy y e^{-y} \frac{(y + iz^2 \frac{\sin tx \sin t}{\sin t} (1-x))^{-3/2}}{\sin t} \right\}$$

For convenience the prime can be dropped and (4.5.9) becomes

$$\rho(E) = \frac{1}{16\pi^2\sqrt{\pi}} \frac{Q^3}{E_Q} \cdot \frac{1}{z} \int_{-\infty}^{\infty} dt (it)^{-3/2} \left(\frac{t}{\sin t}\right)^3 \exp\left\{\frac{3}{2}(t \cot t - 1) - ivz^2 t\right\} \\ - \frac{1}{2} \frac{\xi z^4 t^2}{\pi} \int_0^1 dx \int_0^{\infty} dy e^{-y} \left(y + \frac{iz^2 \sin tx \sin t(1-x)}{\sin t}\right)^{-3/2}$$

4.5.10

Since one is interested in studying the asymptotic behavior of the density of states, one make the transformation $it = T$ or $t = -iT$

$$\sin(-iT) = \frac{\sinh T}{i}, \quad \cos(-iT) = \cosh T$$

$$\sin(iT) = -\frac{\sinh T}{i}, \quad \cot(-iT) = i \coth T$$

$$\frac{iz^2 \sin tx \sin t(1-x)}{\sin t} = \frac{z^2 \sinh T x \sinh T(1-x)}{\sinh T}$$

to get

$$\rho(E) = \frac{1}{16\pi^2\sqrt{\pi}} \frac{1}{z} \frac{Q^3}{E_Q} (-i) \int_{-i\infty}^{i\infty} \frac{dT}{T} \left(\frac{T}{\sinh T}\right)^3 \exp\left\{\frac{3}{2}(T \coth T - 1) - z^2 v T\right\} \\ + \frac{1}{2\sqrt{\pi}} \xi z^4 T^2 \int_0^1 dx \int_0^{\infty} dy e^{-y} \left(y + \frac{z^2 \sinh T x \sinh T(1-x)}{\sinh T}\right)^{-3/2}$$

4.5.11

Sayakanit ³¹ has shown that the above general expression of $\rho(E)$ can be used to obtain the density of states at high energies by letting $t \rightarrow 0$ and the deep tail states by letting $t \rightarrow \infty$.

4.6 The Density of States at High Energy³¹

The path integral method presented previously can be used to obtain the density of states at high and intermediate energies. For states of high energies one may consider the excited state contribution to the density of states by letting $t \rightarrow 0$. For convenience let us write α for z^2 in (4.5.10), then

$$\rho(E) = \frac{1}{16\pi^2} \frac{1}{\sqrt{\alpha}} \frac{Q^3}{E_Q} \int_{-\infty}^{\infty} dt (it)^{-3/2} \left(\frac{t}{\sin t}\right)^3 \exp \left\{ \frac{3}{2} (t \cot t - 1) - i\alpha t \right. \\ \left. - \frac{\alpha^2}{2\sqrt{\pi}} t^2 \int_0^1 dx \int_0^{\alpha} dy y e^{-y} \left(y + \frac{i\alpha \sin t x \sin t (1-x)}{\sin t} \right)^{-3/2} \right\} \quad 4.6.1$$

Eq. (4.6.1) can be changed into series representation by expansion

$$\left(\frac{t}{\sin t}\right)^3 = (t \operatorname{cosec} t)^3 = \left(t \left(\frac{1}{t} + \frac{t}{6} + \dots\right)\right)^3 = \frac{1}{2} + \frac{1}{2} t^2 + \dots \\ t \cot t = t \left(\frac{1}{t} - \frac{t}{3} + \dots\right) = 1 - \frac{t^2}{3} + \dots \\ \frac{\sin t x \sin t (1-x)}{\sin t} = \left(tx - \frac{t^3}{6} x^3 + \dots\right) \left(t(1-x) - \frac{t^3}{6} (1-x)^3 + \dots\right) \left(\frac{1}{t} + \frac{t}{6}\right) \\ = tx(1-x) - \frac{t^3}{6} x(1-x)$$

Thus (4.7.1) may be written as

$$\rho(E) = \frac{1}{16\pi^2} \frac{1}{\sqrt{\alpha}} \frac{Q^3}{E_Q} \int_{-\infty}^{\infty} dt (it)^{-3/2} \left(1 + \frac{1}{2} t^2 + \dots\right) \exp \left\{ \frac{3}{2} \left(1 - \frac{t^2}{3} + \dots - 1\right) \right. \\ \left. - i\alpha t - \frac{\alpha^2}{2\sqrt{\pi}} t^2 \int_0^1 dx \int_0^{\alpha} dy y e^{-y} \left(y + i\alpha \left(tx(1-x) - \frac{t^3}{6} x(1-x) + \dots\right)\right)^{-3/2} \right\} \quad 4.6.2$$

When $t \rightarrow 0$, (4.6.2) becomes

$$\rho(E) = \frac{1}{16\pi^2\sqrt{\pi}} \frac{1}{\sqrt{\alpha}} \frac{Q^3}{E_Q} \int_{-\infty}^{\infty} dt (it)^{-3/2} \exp(-i\alpha vt - \frac{\xi\alpha}{2} t^2) \int_0^{\infty} dx \int_0^{\infty} dy e^{-y/\sqrt{y}} \quad (4.6.3)$$

Since the y -integration can be carried out

$$\int_0^{\infty} dy \sqrt{y}^{-1} e^{-y} = \sqrt{\pi}$$

eq. (4.6.3) becomes

$$\rho(E) = \frac{1}{16\pi^2\sqrt{\pi}} \frac{1}{\sqrt{\alpha}} \frac{Q^3}{E_Q} \int_{-\infty}^{\infty} dt (it)^{-3/2} \exp(-i\alpha vt - \frac{\xi\alpha}{2} t^2) \quad (4.6.4)$$

Eq. (4.6.4) can be expressed in terms of a parabolic-cylinder function by using the formula²²

$$\int_{-\infty}^{\infty} dt (it)^P \exp(-\beta^2 t^2 - iqt) = 2 \frac{-P/2}{\sqrt{\pi}} \beta^{-P-1} \exp(-\frac{q^2}{8\beta^2}) D_P(q/\beta\sqrt{2})$$

Then one has

$$\rho(E) = \frac{1}{16\pi^2\sqrt{\pi}} \frac{1}{\sqrt{\alpha}} \frac{Q^3}{E_Q} \cdot 2 \frac{3/4}{\sqrt{\pi}} (\frac{\alpha}{2})^{1/4} \exp(-\frac{v^2}{4\xi}) D_{-3/2}(\frac{v}{\sqrt{\xi}}) \quad (4.6.5)$$

$$= \frac{2^{3/4}}{16\pi^2} \frac{Q^3}{E_Q^3} \left(\frac{\xi'}{2}\right)^{1/4} \exp\left(-\frac{v^2}{4\xi}\right) D_{-3/2}\left(\frac{v}{\sqrt{\xi}}\right) \quad 4.6.5$$

where $v = \frac{E_0 - E}{E_Q}$, $E_Q = \frac{\hbar^2 Q^2}{2m}$, $\xi = \frac{\xi'}{E_Q^2}$ and

$$\xi' = \frac{2\pi z^2 e^4 n}{Q^2}$$

Let us rewrite (4.6.5) as

$$\rho(E) = \frac{2^{3/4}}{16\pi^2} \frac{Q^3}{E_Q^3} \left(\frac{\xi'}{2E_Q^2}\right)^{1/4} \exp\left(-\frac{(E_0 - E)^2}{4\xi}\right) D_{-3/2}\left(\frac{E_0 - E}{\xi}\right) \quad 4.6.6$$

If we define $\xi' = \frac{\eta^2}{2} = \left(\left\{\frac{4\pi n}{Q}\right\} \cdot \frac{ze^2}{\epsilon_0}\right)^2$, (4.6.6) becomes

$$\rho(E) = \frac{m^{3/2}}{2\pi^2 2^{3/4} \hbar^3} \left(\frac{\eta}{2}\right)^{1/2} \exp\left\{-\frac{(E - E_0)^2}{2\eta^2}\right\} D_{-3/2}\left(\frac{-2(E - E_0)}{\eta}\right) \quad 4.6.7$$

We can study the asymptotic behavior of (4.6.7) by considering the asymptotic expansion of the parabolic cylinder function in (4.6.7) as shown in the following²²

$$D_P(Z) \underset{Z \rightarrow \infty}{\sim} \frac{-\sqrt{2\pi}}{\Gamma(-P)} e^{P\pi i} e^{Z^2/4} Z^{-P-1}$$

where Z is a complex argument. For convenience let us

define $Z = xe^{i\pi}$ and so

$$D_P(-x) \underset{x \rightarrow \infty}{\sim} \frac{\sqrt{2\pi}}{\Gamma(-P)} e^{z^2/4} x^{-P-1} \quad 4.6.8$$

For $z = x$ where μ is real, the asymptotic behavior of a parabolic cylinder function is

$$D_P(x) \underset{x \rightarrow \infty}{\sim} e^{-\frac{x^2}{4}} x^P \quad 4.6.9$$

Thus for $|E_0 - E| \rightarrow \infty$, in the asymptotic limit where

$$\frac{E - E_0}{\eta} \gg 1, \text{ we use (4.6.9) where } x = \frac{\sqrt{2(E - E_0)}}{\eta} \text{ and}$$

replace it into (4.6.7). Eq.(4.6.7) becomes

$$\rho(E) = \frac{m^{3/2}}{\sqrt{2} \pi^2 \hbar^3} \sqrt{E - E_0} \quad 4.6.10$$

This expression is the well known free electron density of states.

Similarly in the asymptotic limit when $\frac{E - E_0}{\eta} \ll -1$, when we can

use (4.6.8) where $x = \frac{\sqrt{2}}{\eta} (E_0 - E)$ and substitute into (4.6.7).

Eq.(4.6.7) becomes

$$\rho(E) = \frac{m^{3/2}}{8\pi^2 \hbar^3} \frac{1}{\eta} \left(\frac{E_0 - E}{\eta} \right)^{-3/2} \exp \left\{ -\frac{|E_0 - E|^2}{2\eta^2} \right\}$$

This expression is the Gaussian band tail familiar to the work of Kane discussed in chapter II.

4.7 The Tail States (low energy) ³¹

We now consider the density of states deep in the tail, ie, in the limit $t \rightarrow \infty$. Since the density of states is the Gaussian form, one can take the limit $t \rightarrow \infty$ the integrated of (4.5.11). We have to look the following terms in series representation

$$\left(\frac{T}{\sinh T}\right)^3 = \left(\frac{2T \cdot e^{-T}}{1 - e^{-2T}}\right)^3 = 8T^3 e^{-3T} (1 - e^{-2T})^{-3}$$

By Binomial series expansion

$$\begin{aligned} &= 8T^3 e^{-3T} \left(\sum_{k=0}^{\infty} \binom{-3}{k} (e^{-2T})^k (-1)^k \right) \\ &= 8T^3 \sum_{k=0}^{\infty} \binom{-3}{k} e^{-T(2k+3)} (-1)^k \end{aligned}$$

where $\binom{-3}{k} = \frac{-3(-3-1)(-3-2) \dots (-3-k+1)}{k!}$

and

$$\begin{aligned} \coth T &= \frac{e^T + e^{-T}}{e^T - e^{-T}} = \frac{1 + e^{-2T}}{1 - e^{-2T}} = \left(1 + \frac{1 + e^{-2T}}{1 - e^{-2T}}\right)^{-1} \\ &= 2(1 - e^{-2T})^{-1} - 1 \\ &= 2 \sum_{k=0}^{\infty} \binom{-1}{k} \cdot e^{-2Tk} \cdot (-1)^k - 1 \end{aligned}$$

Thus

$$\begin{aligned}
 \frac{\sinh Tx \sinh T(1-x)}{\sinh T} &= \frac{1}{2}(1-e^{-2Tx})(1-e^{-2T(1-x)})(1-e^{-2T})^{-1} \\
 &= \frac{1}{2}(1-e^{-2T(1-x)}-e^{-2Tx}+e^{-2T}) \cdot \sum_{k=0}^{\infty} \binom{-1}{k} e^{-2Tk} (-1)^k \\
 &= \frac{1}{2} \left\{ \sum_{k=0}^{\infty} \binom{-1}{k} e^{-2Tk} (-1)^k - \sum_{k=0}^{\infty} \binom{-1}{k} e^{-2T(k+(1-x))} (-1)^k \right. \\
 &\quad \left. - \sum_{k=0}^{\infty} \binom{-1}{k} e^{-2T(k+x)} (-1)^k + \sum_{k=0}^{\infty} \binom{-1}{k} e^{-2T(k+1)} (-1)^k \right\} \\
 &= \frac{1}{2} \left\{ \sum_{k=0}^{\infty} \binom{-1}{k} e^{-2Tk} (-1)^k + \sum_{k=0}^{\infty} \binom{-1}{k} e^{-2T(k+1)} (-1)^k \right\} \\
 &\quad - \frac{1}{2} \left\{ \sum_{k=0}^{\infty} \binom{-1}{k} e^{-2T(k+(1-x))} (-1)^k + \sum_{k=0}^{\infty} \binom{-1}{k} e^{-2T(k+x)} (-1)^k \right\} \\
 &= \frac{1}{2} J(T, x)
 \end{aligned}$$

Thus the series solution of $\rho(E)$ is

$$\begin{aligned}
 \rho(E) &= \frac{1}{16\pi^2 \sqrt{\pi}} \frac{1}{z} \frac{Q^3}{E_Q} (-i) \int_{-i\infty}^{i\infty} \frac{dT}{T^{3/2}} \cdot 8T^3 \sum_{k=0}^{\infty} \binom{-3}{k} (-1)^k e^{-T(2k+3)} \\
 &\quad \cdot \exp \left\{ \frac{3}{2} T \left(2 \sum_{k=0}^{\infty} \binom{-1}{k} e^{-2Tk} (-1)^k - 1 \right) \right. \\
 &\quad \left. - z^2 \nu T + \frac{4}{2\pi} \xi z^4 T^2 \int_0^1 dx \int_0^{\infty} dy e^{-y} \left(y + \frac{z^2}{2} J(T, x) \right)^{-3/2} \right\} \quad 4.7.1
 \end{aligned}$$

Sayakanit considered the ground state contribution to the density of states by letting $t \rightarrow \infty$. The first term of the series dominates and so the density of state $\rho(E)$ becomes

$$\rho(E) = \frac{1}{16\pi^2\sqrt{\pi}} \frac{1}{z} \frac{Q^3}{E_Q} (-i) \int_{-i\infty}^{i\infty} \frac{dT}{3/2} \cdot 8T^3 e^{-3T} \cdot \exp \left\{ \frac{3}{2}(T-1) - z^2 \nu T \right\} \\ + \frac{1}{2\sqrt{\pi}} \xi z^4 T^2 \int_0^1 dx \int_0^\infty dy e^{-y} \cdot y \left(y + \frac{z^2}{2} \right)^{-3/2} \quad 4.7.2$$

This expression can be expressed in a closed form by noting that the y -integration can be expressed in terms of a parabolic cylinder function, ²³ i.e.,

$$\int_0^\infty dy e^{-y} \cdot y \left(y + \frac{z^2}{2} \right)^{-3/2} = 2^{3/2} e^{1/4 z^2} D_{-3}(z)$$

Eq. (4.7.2) can be written as

$$\rho(E) = \frac{1}{2\pi^2\sqrt{\pi}} \frac{1}{z} \frac{Q^3}{E_Q} (-i) \int_{-i\infty}^{i\infty} dT T^{3/2} \exp \left\{ -\left(\frac{3}{2} + z^2 \nu\right) T + \sqrt{\frac{2}{\pi}} \xi z^4 e^{1/4 z^2} D_{-3}(z) T^2 \right\} \\ = \frac{1}{2\pi^2\sqrt{\pi}} \frac{1}{z} \frac{Q^3}{E_Q} \int_{-\infty}^{\infty} dt (it)^{3/2} \exp \left\{ -\left(\frac{3}{2} + z^2 \nu\right) it - \frac{2}{\pi} \xi z^4 e^{1/4 z^2} D_{-3}(z) t^2 \right\}$$

where $T = it$

4.7.3

Eq. (4.7.3) can be performed the t integration by using the formula²²

$$\int_{-\infty}^{\infty} dt (it)^P \exp(-\beta^2 t^2 - iqt) = 2^{-P/2} \sqrt{\pi} \beta^{-P-1} \exp(-q^2/8\beta^2) D_P(q/\beta\sqrt{2})$$

and so the density of states is

$$\rho(v, z) = \frac{2^{-3/4}}{2\pi^2 \sqrt{\pi}} \frac{1}{z} \frac{Q^3}{E_Q} \sqrt{\pi} \beta^{-5/2} \exp(-(\frac{3/2 + z^2 v}{8\beta^2})^2) D_{3/2}(\frac{3/2 + z^2 v}{\sqrt{2} \beta}) \quad 4.7.4$$

$$\text{where } \beta^2 = \frac{2}{\pi} \xi z^4 e^{1/4 z^2} D_{-3/2}(z)$$

The above expression can be expressed in closed form

$$a(v, z) = (\frac{3/2 + z^2 v}{8\pi\sqrt{2}})^{3/2} z^6 \exp(z^2/2) D_{-3/2}^2(z) \quad 4.7.5$$

and

$$b(v, z) = (\frac{3/2 + z^2 v}{2\sqrt{2}})^2 \sqrt{\pi} / 2 \exp(z^2/2) D_{-3/2}(z) \quad 4.7.6$$

Eq. (4.7.4) can then be rewritten as

$$\rho_1(v, z) = \frac{Q^3}{E_Q \xi^{5/4}} \frac{a(v, z)}{b(v, z)^{3/4}} e^{-\frac{b(v, z)}{4\xi}} D_{3/2}(\sqrt{\frac{b(v, z)}{\xi}}) \quad 4.7.7$$

In the limit of large $b(v, z) / \xi$ the asymptotic expression for the parabolic cylinder function is

$$D_p(X) = e^{-X^2/4} X^p (1 - \frac{p(p-1)}{2} \frac{1}{X^2} + \dots) \quad 4.7.8$$

If we neglect the term in X^{-2} in (4.7.8), we obtain

$$\rho(v, z) = \frac{Q^3}{E_Q \xi^2} a(v, z) e^{-\frac{b(v, z)}{2\xi}} \quad 4.7.9$$

Sayakanit followed the procedure of Halperin and Lax to obtain, the best choice of z . As pointed out by Halperin and Lax, one can reach the low energy tail in two equivalent ways by letting $E \rightarrow -\infty$ or keeping E constant and reducing the magnitude of the potential fluctuation by letting $\xi \rightarrow 0$. In Halperin and Lax's limit ($\xi \rightarrow 0$) the exponential factor of (4.7.9) will dominate and become very sensitive to the choice of z while other factors are much more slowly varying. Hence one can follow the procedure of Halperin and Lax (chapter 3) that is we maximize the exponential term of (4.7.9) by considering

$$\frac{\delta}{\delta z} \exp\left(-\frac{b(v,z)}{2\xi}\right) = 0 \quad 4.7.10$$

where

$$\begin{aligned} \frac{\delta b(v,z)}{\delta z} &= \frac{\pi}{2\sqrt{2}} \frac{d}{dz} \left[\frac{1}{2\xi z^4} \frac{(3/2+z^2v)^2}{\exp(z^2/4)} D_{-3}(z) \right] \\ &= -3b(v,z)z \left\{ \frac{2}{z(3/2+z^2v)} - \frac{D_{-4}(z)}{D_{-3}(z)} \right\} \end{aligned} \quad 4.7.11$$

To obtain the above result we have used the relation

$$\frac{d}{dz} D_{-3}(z) = -3D_{-4}(z) - \frac{1}{2}zD_{-3}(z)$$

Setting the left side of (4.7.11) to zero, we obtain

$$D_{-3}(z) = \frac{z^3}{2} \left(\frac{3}{2z} 2^{+v} \right) D_{-4}(z) \quad 4.7.12$$

The best choice of z is that which satisfies (4.7.12). The value of z

that is obtained for each values of v will be substituted into (4.7.9) and the value of $\rho(E)$ for each v can be obtained. Sayakanit (1977) has shown in his numerical results that they correspond to Halperin and Lax 's result. Since Sayakanit has obtained the analytic expression of $\rho(E)$, one can study analytically the limiting values of $a(v)$, $b(v)$, $n(v)$, and $T(v)$. We shall study in two cases.

The strong screening cases.

For the case of strong screening ($Q \rightarrow \infty$) which is equivalent to $v \ll 1$ or $z \rightarrow \infty$, the asymptotic form of parabolic cylinder functions are

$$D_{-3}(z) \underset{z \rightarrow \infty}{\approx} e^{-z^2/4} / z^3 \quad 4.7.13$$

and

$$D_{-4}(z) \underset{z \rightarrow \infty}{\approx} e^{-z^2/4} / z^4 \quad 4.7.14$$

Substituting (4.7.13) and (4.7.14) into (4.7.12), we get for limiting value of z

$$z = \sqrt{\frac{1}{2v}} \quad 4.7.15$$

Substituting (4.7.13) and (4.7.14) into (4.7.6), one gets the limiting values of

$$\begin{aligned} b(v, z) &= (2v)^{1/2} \frac{\sqrt{\pi}}{2\sqrt{2}} \left(\frac{3}{2} + \frac{v}{2v}\right)^2 \\ &= 2\sqrt{\pi} v^{1/2} \end{aligned} \quad 4.7.16$$

Substituting (4.7.13) and (4.7.14) into (4.7.5), one obtains the limiting values of

$$a(v, z) = v^{3/2} / \sqrt{2} \pi \quad 4.7.17$$

The kinetic energy of localization $T(v)$, can be obtained from the term $b(v, z)$, i.e.,

$$T(v) = \frac{3}{2z^2} \quad 4.7.18$$

The limiting value of $T(v)$ can be obtained by substituting the limiting value of z in (4.7.18), we get

$$\frac{T(v)}{v} = \frac{3}{2} \cdot \frac{2v}{v} \sim 3 \quad 4.7.19$$

Besides the dimensionless functions $a(v)$, $b(v)$, and $T(v)$ other quantities of interest are the logarithmic derivative of the exponent $b(v, z)$, i.e.,

$$\begin{aligned} n(v) &= d \log(b, z) / d \log v \\ &= \frac{v}{b(v, z)} \cdot \frac{\partial b(v, z)}{\partial v} \end{aligned} \quad 4.7.20$$

For obtaining $n(v)$, (4.7.6) can be differentiated and substituted into (4.7.20) we have

$$n(v) = \frac{v \cdot 2\sqrt{2} e^{1/4 z^2} D_{-3}(z) \cdot 2 \sqrt{\pi} (\frac{3}{2z^2} + v)}{\sqrt{\pi} (\frac{3}{2z^2} + v)^2 \cdot 2\sqrt{2} \exp(\frac{z^2}{4}) D_{-3}(z)}$$

$$= 2v / \left(\frac{3}{2} z^2 + v \right) \quad 4.7.21$$

To obtain, the limiting value of $n(v)$ for this case, the limiting value of z will be substituted into (4.7.21)

$$\begin{aligned} n(v) &\approx 2v / (3v + v) \\ &= \frac{1}{2} \end{aligned}$$

The weak screening

In the limit which $v \gg 1$. ($Q \rightarrow 0$ or $z \rightarrow 0$), where the asymptotic forms of the parabolic cylinder function are

$$\begin{aligned} D_{-3}(z) \\ z \rightarrow 0 \end{aligned} = \frac{1}{2} \sqrt{\frac{1}{2} \pi} \quad 4.7.22$$

$$\begin{aligned} D_{-4}(z) \\ z \rightarrow 0 \end{aligned} = \frac{1}{3} \quad 4.7.23$$

Using (4.7.12) one obtains for the limiting value of z

$$\begin{aligned} \frac{1}{2} \sqrt{\frac{1}{2} \pi} &= \frac{1}{6} z^3 \left(\frac{3}{2} z^{-2} + v \right) \\ z &\approx \left(3 \sqrt{\frac{1}{2} \pi} \right)^{1/3} v^{-1/3} \end{aligned} \quad 4.7.24$$

where one used the approximation $z^{-2} \ll v$

Similarly the limiting values $a(v)$, $b(v)$, $T(v)$, $n(v)$ for this case can be obtained by substituting (4.7.22) and (4.7.23) into (4.7.5),

(4.7.18) and (4.7.21) respectively. Thus we obtain the following.

$$a(v, z) = \frac{\left(\frac{3}{2}z^2 + v\right)^{3/2}}{8\pi\sqrt{2} \left(\frac{9}{2}\pi\right)v^{-2} \cdot \frac{1}{8\pi}}$$

$$= \frac{v^{3/2}}{8\pi\sqrt{2} \left(\frac{9}{2}\pi\right)v^{-2} \cdot \frac{1}{8\pi}}$$

$$= \frac{\sqrt{2}}{9\pi^3} v^{7/2}$$

$$b(v, z) = \frac{\sqrt{\pi} \left(\frac{3}{2}z^2 + v\right)^2}{2\sqrt{2} \exp\left(\frac{z^2}{4}\right) D_{-3}(z)}$$

$$= \frac{\sqrt{\pi} v^2}{2\sqrt{2} \left(\frac{1}{2} \sqrt{\frac{1}{2}} \pi\right)}$$

$$= 2$$

$$n(v) \approx \frac{2v}{v}$$

$$= 2$$

and

$$\frac{T(v)}{v} = \frac{3}{2} 2^{-1/3} v^{-1/3}$$

$$\approx \frac{3}{2} \left(\frac{3\sqrt{1\pi}}{2} \right)^{1/3} \frac{v}{v} = 0 \quad (v \gg 1)$$

For comparison, it is interesting to note that the path integral method and the method of Halperin and Lax give the identical limiting values for $n(v)$ and $\frac{T(v)}{v}$ but slightly different values for $a(v)$ and $b(v)$ as shown in Table 4.1

	$v \ll 1$	$v \gg 1$
$a(v)$	$\approx \frac{1}{\sqrt{2\pi}} v^{3/2} \approx 0.23 v^{3/2} (\approx 0.4 v^{3/2})$	$\approx \frac{2}{(9\pi)^3} v^{7/2} \approx 0.5 \times 10^{-2} v^{7/2} (\approx 10^{-2} v^{7/2})$
$b(v)$	$\approx 2\sqrt{\pi} v^{1/2} \approx 3.54 v^{1/2} (\approx 3 v^{1/2})$	$\approx v^2 (\approx v^2)$
$n(v)$	$\approx \frac{1}{2} (\approx \frac{1}{2})$	$\approx 2 (\approx 2)$
$\frac{T(v)}{v}$	$\approx 3 (\approx 3)$	$\approx 0 (\approx 0)$

Table 4.1 Comparison between the limiting values of $a(v)$, $b(v)$, $n(v)$ and $\frac{T(v)}{v}$ calculated from the path integral method and the method of Halperin and Lax for the case of screened coulomb potential. The values within the parentheses are those of Halperin and Lax (Table 3.1)

Sayakanit obtained the analytic form of $\rho(E)$ and showed also that Halperin and Lax's density of states and Kane's density of states were the limiting cases ($t \rightarrow 0$, $t \rightarrow \infty$) of his general expression $\rho(E)$. He pointed out that his result could be extended to intermediate energies. He also pointed out that Halperin and Lax's limit did not satisfy to the variation principle. To understand the failure of Halperin and Lax's limit let us consider Fig 3.2. We can see that there is an unphysical region ($v \ll 1$). To remove this region Sa-yakanit suggested that one might use the Lloyd and Best variational principle.