

Chapter 3

Heavily Doped Strongly Compensated Semiconductors Model

This chapter we provide a model of heavily doped strongly compensated semiconductors (HDCS) [9,20,40]. We begin the study by modelling HDCS as an electron moving in a large number of impurities in a disordered system by using Edwards' model [5,6,25]. In the second section, the autocorrelation function which is important in the disordered system is presented. Next, we will present our density of states (DOS). In the last section, the trial propagator is given.

3.1 Edwards' Model

Firstly, we consider an electron moving in a set of N rigid scatterers confined within a volume V and having a density $\bar{N} = N/V$. Such a system is described by the Hamiltonian $H[v]$ [6,25],

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

where $v(\vec{x}(\tau) - \vec{R}_i)$ represents the potential of a single scatterer at position \vec{R}_i .

The time-dependent Schrödinger like equation for an electron of the effective mass m in a disordered system which is

$$\left[i\hbar \frac{\partial}{\partial t} - H[v] \right] K(\vec{x}_2, \vec{x}_1; t, [v]) = \delta(\vec{x}_2 - \vec{x}_1) \delta(t). \quad (3.2)$$

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

$$K(\vec{x}_2, \vec{x}_1; t, [v]) = \int D[\vec{x}(\tau)] \exp \left(\frac{i}{\hbar} \int_0^t d\tau \left[\frac{m}{2} \dot{\vec{x}}^2(\tau) - v(\vec{x}(\tau) - [\vec{R}]) \right] \right), \quad (3.3)$$

where $D[\vec{x}(\tau)]$ denotes the path integrals to be carried out with the boundary conditions: $\vec{x}(0) = \vec{x}_1$ and $\vec{x}(t) = \vec{x}_2$. We denote $v(\vec{x}(\tau) - [\vec{R}])$ as the sum of the scattering potentials, i.e.

$$v(\vec{x}(\tau) - [\vec{R}]) = \sum_i v(\vec{x}(\tau) - \vec{R}_i). \quad (3.4)$$

The probability distribution of the scattering potentials is assumed to be

$$P[\vec{R}]d([\vec{R}]) = \prod_{N, V \rightarrow \infty} \frac{d\vec{R}_1, \dots, d\vec{R}_N}{V^N}. \quad (3.5)$$

In 1964, Edwards and Gulyaev [6] pointed out that the average over all configurations in Eq. (3.3) can be performed exactly and the result is

$$K(\vec{x}_2, \vec{x}_1; t) = \int P[\vec{R}]d([\vec{R}])K(\vec{x}_2, \vec{x}_1; t, [V]). \quad (3.6)$$

Substituting Eq. (3.5) into Eq. (3.6), we have

$$K(\vec{x}_2, \vec{x}_1; t) = \int_{N, V \rightarrow \infty} \prod \frac{d\vec{R}_1, \dots, d\vec{R}_N}{V^N} K(\vec{x}_2, \vec{x}_1; t, [V]), \quad (3.7)$$

where V is a volume of the semiconductor. By using Eq. (3.3), we get

$$K(\vec{x}_2, \vec{x}_1; t) = \int_{N, V \rightarrow \infty} \prod \frac{d\vec{R}_1, \dots, d\vec{R}_N}{V^N} \int D[\vec{x}(\tau)] \times \exp \left(\frac{i}{\hbar} \int_0^t d\tau \left[\frac{m}{2} \dot{\vec{x}}^2(\tau) - v(\vec{x}(\tau) - [\vec{R}]) \right] \right). \quad (3.8)$$

Then Eq. (3.6) can be rewritten as

$$K(\vec{x}_2, \vec{x}_1; t) = \int D[\vec{x}(\tau)] \exp \left\{ \frac{i}{\hbar} \int_0^t d\tau \frac{m}{2} \dot{\vec{x}}^2(\tau) + \bar{N} \int d\vec{R} \left[\exp \left(-\frac{i}{\hbar} \int d\tau v(\vec{x}(\tau) - \vec{R}) \right) - 1 \right] \right\}. \quad (3.9)$$

By using the relation

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots, \quad (3.10)$$

the term inside the square brackets of Eq. (3.9) can be written as

$$\exp \left(-\frac{i}{\hbar} \int d\tau v(\vec{x}(\tau) - \vec{R}) \right) - 1 = \left[1 - \frac{i}{\hbar} \int_0^t d\tau v(\vec{x}(\tau) - \vec{R}) - \frac{1}{2\hbar^2} \int_0^t d\tau v(\vec{x}(\tau) - \vec{R}) \int_0^t d\tau v(\vec{x}(\tau) - \vec{R}) - \dots \right] - 1. \quad (3.11)$$

So that, Eq. (3.9) becomes

$$K(\vec{x}_2, \vec{x}_1; t) = \int D[\vec{x}(\tau)] \exp \left\{ \frac{i}{\hbar} \int_0^t d\tau \frac{m}{2} \dot{\vec{x}}^2(\tau) + \bar{N} \int d\vec{R} \left[\left(1 - \frac{i}{\hbar} \int_0^t d\tau v(\vec{x}(\tau) - \vec{R}) - \frac{1}{2\hbar^2} \int_0^t d\tau v(\vec{x}(\tau) - \vec{R}) \int_0^t d\tau v(\vec{x}(\tau) - \vec{R}) - \dots \right) - 1 \right] \right\}. \quad (3.12)$$

In the limits of high density, $\bar{N} \rightarrow \infty$, and weak scatterer, $v \rightarrow 0$ with $\bar{N}v^2$ remains finite, Eq.(3.12) can be simplified to

$$K(\vec{x}_2, \vec{x}_1; t) = \int D[\vec{x}(\tau)] \exp \left[\frac{i}{\hbar} \int_0^t d\tau \frac{m}{2} \dot{\vec{x}}^2(\tau) - \frac{\bar{N}\eta^2}{2\hbar^2} \int_0^t \int_0^t d\tau d\sigma W(\vec{x}(\tau) - \vec{x}(\sigma)) \right], \quad (3.13)$$

where the mean potential energy has been taken as zero and W denotes the autocorrelation function [25] defined as

$$W(\vec{x}(\tau) - \vec{x}(\sigma)) = \int d\vec{R} v(\vec{x}(\tau) - \vec{R}) v(\vec{x}(\sigma) - \vec{R}). \quad (3.14)$$

The autocorrelation function is an important function because it tells us the effect of a potential at one point on a potential at another point. The parameter η , denoting the weakness of the scattering potential, is explicitly written here to indicate the dimensions involved. The average propagator in Eq. (3.13) can be formally expressed in terms of an action S as

$$K(\vec{x}_2, \vec{x}_1; t) = \int D[\vec{x}(\tau)] \exp \left(\frac{i}{\hbar} S \right), \quad (3.15)$$

where S is defined by

$$S = \int_0^t d\tau \frac{m}{2} \dot{\vec{x}}^2(\tau) + \frac{i}{2\hbar} \bar{N}\eta^2 \int_0^t \int_0^t d\tau d\sigma W(\vec{x}(\tau) - \vec{x}(\sigma)). \quad (3.16)$$

Thus we have given in this section a brief discussion of Edwards' model and have set $\bar{N}\eta^2 = 1$ [25]. The autocorrelation function W defined by Eq. (3.14) clearly depends on the scattering potential employed. For a screened Coulomb scattering potential of the form

$$v(\vec{x}(\tau) - \vec{R}) = \frac{\exp(-\alpha |\vec{x}(\tau) - \vec{R}|)}{|\vec{x}(\tau) - \vec{R}|}, \quad (3.17)$$

where α is a constant. It follows from Eqs. (3.14) and (3.17) that the autocorrelation [25] is

$$W(\vec{x}(\tau) - \vec{x}(\sigma)) = \int \frac{d\vec{q}}{(2\pi)^3} \left(\frac{4\pi}{q^2 + \alpha^2} \right)^2 \exp[i\vec{q} \cdot (\vec{x}(\tau) - \vec{x}(\sigma))], \quad (3.18)$$

which is expressed as the Fourier transform of the screened Coulomb scattering potential.

3.2 The Autocorrelation Function

In this thesis, we consider the autocorrelation function [40] given by

$$W(\vec{x}(\tau) - \vec{x}(\sigma)) = W_1(\vec{x}(\tau) - \vec{x}(\sigma)) + W_2(\vec{x}(\tau) - \vec{x}(\sigma)), \quad (3.19)$$

where

$$W_1(\vec{x}(\tau) - \vec{x}(\sigma)) = \frac{2\pi\gamma^2}{r_0} \int \frac{d^3q}{(2\pi)^3} \frac{\exp[i\vec{q} \cdot (\vec{x}(\tau) - \vec{x}(\sigma))]}{q^2 (q^2 + r_e^{-2} + r_0^{-2})}, \quad (3.20)$$

and

$$W_2(\vec{x}(\tau) - \vec{x}(\sigma)) = \frac{2\pi\gamma^2}{r_0} \int \frac{d^3q}{(2\pi)^3} \frac{r_e^{-2} \exp[i\vec{q} \cdot (\vec{x}(\tau) - \vec{x}(\sigma))]}{q^4 (q^2 + r_e^{-2} + r_0^{-2})}, \quad (3.21)$$

where

$$\gamma = \frac{e^2 (N_T r_0^3)^{1/2}}{2\sqrt{\pi} \epsilon_0 K r_0} \quad (3.22)$$

is the root-mean-squared potential created by a typical fluctuation of size r_0 ,

$$r_0 = \left(\frac{\epsilon_0 K k T_0}{N_T e^2} \right)^{1/2} \quad (3.23)$$

is the distance which leads to an ionic screening of the potential,

$$r_e = \left(\frac{\epsilon_0 K k T_0}{2pe^2} \right)^{1/2} \quad (3.24)$$

is the Debye screening length which takes into account the presence of the intrinsic electrons and holes with concentration $2p$ at the temperature T_0 . It should

be noted that e is the electron charge, $N_T = N_D + N_A$ is the total impurity concentration, N_D is donor impurity density, N_A is acceptor impurity density, ϵ_0 is the dielectric constant of a pure semiconductor, K is the static dielectric

constant and k is the Boltzmann constant. Substituting Eqs. (3.20) and (3.21) into Eq. (3.19) we obtain

$$W(\vec{x}(\tau) - \vec{x}(\sigma)) = \frac{2\pi\gamma^2}{r_0} \int \frac{d^3q}{(2\pi)^3} \frac{\exp[i\vec{q} \cdot (\vec{x}(\tau) - \vec{x}(\sigma))]}{q^2 (q^2 + r_e^{-2} + r_0^{-2})} + \frac{2\pi\gamma^2}{r_0} \int \frac{d^3q}{(2\pi)^3} \frac{r_e^{-2} \exp[i\vec{q} \cdot (\vec{x}(\tau) - \vec{x}(\sigma))]}{q^4 (q^2 + r_e^{-2} + r_0^{-2})}, \quad (3.25)$$

which is expressed as the Fourier transform.

3.3 The Density of States

The most used form of the density of states [12] is

$$\rho(E) = \frac{1}{V} \left\langle \sum_i \delta(E - E_i) \right\rangle, \quad (3.26)$$

where $\delta(x)$ is the Dirac delta function, E_i is the energy of the i^{th} eigenstates of a Hamiltonian, V is a container of N scatterers in d dimensions, and the angular bracket $\langle \dots \rangle$ indicates an average over the ensemble of the scatterer positions. In our work, we use the formula in Eq. (3.26) because the Dirac delta function can be expressed in terms of a transformed propagator. With the energy expansion formula of the propagator [8,24],

$$K(\vec{x}_2, \vec{x}_1; t) = \sum_i \varphi_i(\vec{x}_2) \varphi_i^*(\vec{x}_1) \exp\left[-\frac{iE_i t}{\hbar}\right], \quad (3.27)$$

where $\varphi_i(\vec{x})$ is the wavefunction, we have the trace of the propagator of the form:

$$\text{Tr}K(\vec{x}_2, \vec{x}_1; t) = \sum_i \exp \left[-\frac{iE_i t}{\hbar} \right]. \quad (3.28)$$

By taking a Fourier transform of both sides of Eq. (3.28), one obtains

$$\int_{-\infty}^{+\infty} dt \text{Tr}K(\vec{x}_2, \vec{x}_1; t) \exp \left[\frac{iEt}{\hbar} \right] = 2\pi\hbar \sum_i \delta(E - E_i). \quad (3.29)$$

Note that the identities,

$$\delta(a) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \exp[iax] dx, \quad (3.30)$$

and

$$\delta\left(\frac{a}{b}\right) = b\delta(a), \quad (3.31)$$

are used in the derivation of Eq. (3.29). Now the required relation between the density of states and the propagator is obtained by comparing Eq. (3.26) with Eq. (3.29), and performing the Fourier transform according to the standard formula [25]

$$\rho(E) = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dt \text{Tr}K(\vec{x}_2, \vec{x}_1; t) \exp \left[\frac{iEt}{\hbar} \right]. \quad (3.32)$$

For heavily doped strongly compensated semiconductors, as already mentioned, the propagator in Eq. (3.32) must be the average propagator instead. That is, the density of states of our problem has the following form:

$$\rho(E) = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dt \text{Tr}\bar{K}(\vec{x}_2, \vec{x}_1; t) \exp \left[\frac{iEt}{\hbar} \right], \quad (3.33)$$

where \bar{K} is obtained by averaging over all configurations of scatterers, and it must have the property [25]

$$\bar{K}(\vec{x}_2, \vec{x}_1; t) = \bar{K}(\vec{x}_2 - \vec{x}_1; t). \quad (3.34)$$

For simplicity in writing, we will write $K(\vec{x}_2, \vec{x}_1; t)$ instead of $\bar{K}(\vec{x}_2, \vec{x}_1; t)$. Eq. (3.33) can be rewritten as follows:

$$\rho(E) = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dt \text{Tr} K(\vec{x}_2, \vec{x}_1; t) \exp \left[\frac{iEt}{\hbar} \right], \quad (3.35)$$

which involves only the diagonal part of K . The density of states per unit volume can be derived from the diagonal part of the averaged propagator [40], so that

$$\rho(E) = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dt K(0, 0; t) \exp \left[\frac{i}{\hbar} Et \right]. \quad (3.36)$$

3.4 The Variational Method

In this section, we discuss a method based on the variational principle [8] for the approximate evaluation of certain path integrals. We consider those problems for which the method may be useful. The average value of e^x , when x is a random variable in an one dimensional, always exceeds or equals to the exponential of the average value of x , as long as x is real and the weights used in the averaging process are positive. That is

$$\langle e^x \rangle \geq e^{\langle x \rangle}, \quad (3.37)$$

where $\langle x \rangle$ is the weighted average of x . This follows from the fact that the curve of e^x is concave upward, as shown in Figure 3.1. If a number of masses (weights) lie along this curve, the center of gravity of these masses lies above the curve. The vertical height of this center of gravity is the average vertical position $\langle e^x \rangle$ of the points. It exceeds $e^{\langle x \rangle}$, the ordinate of the curve e^x at the abscissa position of the center of gravity, which is the average value $\langle x \rangle$.

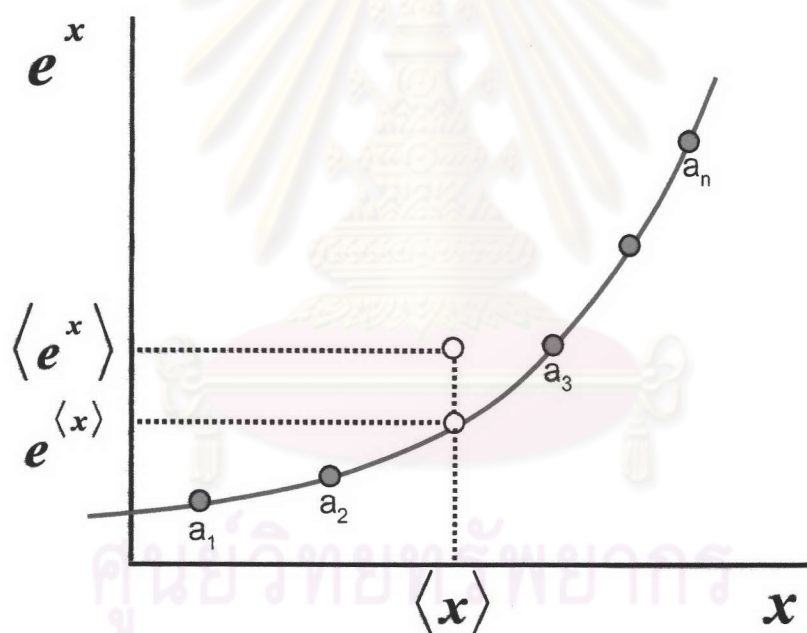


Figure 3.1 The exponential of the weighted average of x , $e^{\langle x \rangle}$, must lie below the weighted average of the exponentials $\langle e^x \rangle$. The value of $e^{\langle x \rangle}$ must lie in the curve, but $\langle e^x \rangle$, the center of gravity of the several points, must lie above the curve [8].

3.5 The Trial Propagator

In order to calculate the propagator of the trial system which is represented by the trial action, we shall follow the standard method. Firstly considering the classical action Eq. (2.18), we can see that

$$S_{cl}[\vec{x}_2, \vec{x}_1; t, \omega] = S[\vec{x}(t)] = S[\vec{x}_{cl}(t)]. \quad (3.38)$$

We will try to write an equation similar to Eq. (2.20) in Chapter 2

$$S[\vec{x}(t)] = S_{cl}[\vec{x}_2, \vec{x}_1; t, \omega] + \int_a^b \left[a(t) \dot{\vec{y}}^2 + b(t) \dot{\vec{y}} \cdot \vec{y} + c(t) \vec{y}^2 \right] dt. \quad (3.39)$$

Starting from the trial action [25]

$$S_0(\omega) = \int_0^t d\tau \frac{m}{2} \dot{\vec{x}}^2(\tau) - \frac{m\omega^2}{4t} \int_0^t \int_0^t d\tau d\sigma [\vec{x}(\tau) - \vec{x}(\sigma)]^2 \quad (3.40)$$

and using the formula $S[\vec{x}(t)] = S[\vec{x}(t) + \vec{y}(t)] = S[\vec{x}_{cl}(t) + \vec{y}(t)]$, we get

$$\begin{aligned} S_0[\vec{x}(t)] &= \int_0^t d\tau \frac{m}{2} \dot{\vec{x}}_{cl}^2(\tau) + \int_0^t d\tau m \dot{\vec{x}}_{cl}(\tau) \cdot \dot{\vec{y}}(\tau) + \int_0^t d\tau \frac{m}{2} \dot{\vec{y}}^2(\tau) \\ &\quad - \frac{m\omega^2}{4t} \int_0^t \int_0^t d\tau d\sigma [\vec{x}_{cl}(\tau) - \vec{x}_{cl}(\sigma)]^2 \\ &\quad - \frac{m\omega^2}{2t} \int_0^t \int_0^t d\tau d\sigma [\vec{x}_{cl}(\tau) - \vec{x}_{cl}(\sigma)] \cdot [\vec{y}(\tau) - \vec{y}(\sigma)] \\ &\quad - \frac{m\omega^2}{4t} \int_0^t \int_0^t d\tau d\sigma [\vec{y}(\tau) - \vec{y}(\sigma)]^2. \end{aligned} \quad (3.41)$$

Using the approximation in Eq.(3.41) and ignoring the second order term of variable y , we obtain

$$S_0 [\vec{x}(t)] = S_0 [\vec{x}_{cl}(t)] + \int_0^t d\tau m \dot{\vec{x}}_{cl}(\tau) \cdot \dot{\vec{y}}(\tau) - \frac{m\omega^2}{2t} \int_0^t \int_0^t d\tau d\sigma [\vec{x}_{cl}(\tau) - \vec{x}_{cl}(\sigma)] \cdot [\vec{y}(\tau) - \vec{y}(\sigma)], \quad (3.42)$$

where we write the classical action as

$$S_0 [\vec{x}_{cl}(t)] = \int_0^t d\tau \frac{m}{2} \dot{\vec{x}}_{cl}^2(\tau) - \frac{m\omega^2}{4t} \int_0^t \int_0^t d\tau d\sigma [\vec{x}_{cl}(\tau) - \vec{x}_{cl}(\sigma)]^2. \quad (3.43)$$

We can see the classical action in Eq. (3.43) is exactly the same as the trial action in Eq. (3.40). Comparing Eq. (3.39) with Eq. (3.42) we obtain

$$S_0 [\vec{x}_{cl}(t)] = S_{0,cl} [\vec{x}_2, \vec{x}_1; t, \omega]. \quad (3.44)$$

The trial propagator enables us to separate the path integrals into two parts: one is the classical contribution and the other is the fluctuation or quantum contribution [8], called the prefactor or multiplicative factor. In certain systems, the prefactor depends only on the flight time. Hence, such a propagator [25] can be written as

$$K_0 (\vec{x}_2, \vec{x}_1; t, \omega) = F(t, \omega) \exp \left[\frac{i}{\hbar} S_{0,cl} [\vec{x}_2, \vec{x}_1; t, \omega] \right], \quad (3.45)$$

where $F(t, \omega)$ is the prefactor which must be determined so that for $\omega \rightarrow 0$,

$$F(t) = \left(\frac{m}{2\pi i \hbar t} \right)^{\frac{3}{2}}. \quad (3.46)$$

We can obtain the prefactor by considering the trial action $S_0(\omega)$ obtained from a simple harmonic oscillator propagator [25]

$$\mathcal{L}(\vec{x}_2, \vec{x}_1; t, \vec{y}) = \int D[\vec{x}(\tau)] \exp\left(\frac{i}{\hbar} \int_0^t d\tau \left[\frac{m}{2} \dot{\vec{x}}^2(\tau) - \frac{\kappa}{2} |\vec{x}(\tau) - \vec{y}|^2 \right]\right), \quad (3.47)$$

where \vec{y} is the origin of the harmonic oscillator and κ is the force constant. Next, we simply integrate Eq. (3.47) with respect to \vec{y}

$$\begin{aligned} K(\vec{x}_2, \vec{x}_1; t, \omega) &= \int d\vec{y} \mathcal{L}(\vec{x}_2, \vec{x}_1; t, \vec{y}) \\ &= \left(\frac{\pi\hbar}{i\kappa}\right)^{\frac{3}{2}} \int D[\vec{x}(\tau)] \exp\left(\frac{i}{\hbar} S_0(\omega)\right), \end{aligned} \quad (3.48)$$

where $\omega = (\kappa/m)^{1/2}$ denotes the frequency of a harmonic oscillator. Next, we consider the next integral of the delta function using the partition function. From Feynman and Hibbs' book [8], Eq. (3.48) can be rewritten as

$$\begin{aligned} \int d\vec{x}_1 \int d\vec{x}_2 K(\vec{x}_2, \vec{x}_1; t, \omega) \delta(\vec{x}_2 - \vec{x}_1) &= \int d\vec{y} \int d\vec{x}_1 \int d\vec{x}_2 \mathcal{L}(\vec{x}_2, \vec{x}_1; t, \vec{y}) \delta(\vec{x}_2 - \vec{x}_1) \\ &= U \left(2i \sin \frac{1}{2}\omega t\right)^{-3}. \end{aligned} \quad (3.49)$$

The first equality of the above expression is obtained by using the first equality of expression Eq. (3.48) with the integrals interchanged. Apart from the factor U , the second equality of Eq. (3.49) is the partition function of a simple harmonic oscillator. Similarly the “partition function” [8,25] corresponding to $K_0(\vec{x}_2, \vec{x}_1; t, \omega)$ is

$$\int d\vec{x}_1 \int d\vec{x}_2 K_0(\vec{x}_2, \vec{x}_1; t, \omega) \delta(\vec{x}_2 - \vec{x}_1) = UF(t, \omega). \quad (3.50)$$

Since $K_0(\vec{x}_2, \vec{x}_1; t, \omega)$ and $K(\vec{x}_2, \vec{x}_1; t, \omega)$ differ only by a constant, their corresponding partition functions must differ by constant too. Therefore, we can equate Eq. (3.50) to Eq. (3.49) with a constant C

$$UF(t, \omega) = CU \left(2i \sin \frac{1}{2} \omega t \right)^{-3}. \quad (3.51)$$

Using the boundary condition of the prefactor $F(t)$ discussed earlier in Eqs. (3.46) and (3.51), we have

$$F(t, \omega) = \left(\frac{m}{2\pi i \hbar t} \right)^{\frac{3}{2}} \left(\frac{\omega t}{2 \sin \frac{1}{2} \omega t} \right)^3. \quad (3.52)$$

We can put Eq. (3.52) back into Eq. (3.45) to obtain the propagator of the classical action Eq. (3.43). The calculation of the density of states will be presented in the next chapter.

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