

CHAPTER II

A HEAVILY DOPED SEMICONDUCTOR MODEL

A MODELLED HAMILTONIAN

Starting from the “first principle” and the effective mass approximation, the Hamiltonian of a heavily doped semiconductor can be written as

$$H = \sum_i \frac{1}{2} m \dot{x}_i^2 + \sum_{i,j} \frac{Ze^2}{|\mathbf{x}_i - \mathbf{x}'_j|} + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{\epsilon_0 |\mathbf{x}_i - \mathbf{x}_j|}, \quad (2.1)$$

where \mathbf{x}, \mathbf{x}' are the positions of an electron and of an impurity, respectively, m is the effective mass of an electron moving in a pure semiconductor, ϵ_0 the dielectric constant of a pure semiconductor, and Z an atomic number of impurity. Note that, for simplicity, only one kind of impurities is doped into a semiconductor randomly. Of course, this Hamiltonian is a reduced form of the full many-body Hamiltonian under the Born-Oppenheimer approximation. Wolff (1962) tried to work out this problem within a lowest-order perturbation theory. It is found that the electron-electron interactions are to screen the electron-impurity interactions and shift the conduction band nearly rigid downward. In fact, there is a band tail due to the electron-electron interactions, but it is small (Berggren and Sernelius, 1981). Since we are interested in the band tailing, the one electron approximation, neglecting the electron-electron

interactions, is sufficient for the following discussions. That is, only the randomness of doping impurities, not the many-body one, shall be studied.

From above discussion, we can say that a heavily doped semiconductor should be modelled as a system of an electron moving in a large number of impurities. The one-electron Hamiltonian can then be written as

$$H = \frac{1}{2}m\dot{\mathbf{x}}^2 + \sum_{i=1}^N v(\mathbf{x} - \mathbf{x}'_i), \quad (2.2)$$

where N is a number of impurities. This Hamiltonian seems very simple but it provides us sufficient information. Two types of potentials $v(\mathbf{x} - \mathbf{x}')$ seen by an electron due to an impurity at point \mathbf{x}' are considered; one is the Gaussian potential given by

$$v(\mathbf{x} - \mathbf{x}') = u(\pi l^2)^{-\frac{1}{2}} \exp\left[-\frac{|\mathbf{x} - \mathbf{x}'|^2}{l^2}\right], \quad (2.3)$$

and another is the screened Coulomb one,

$$v(\mathbf{x} - \mathbf{x}') = \frac{Ze^2}{\epsilon_0 |\mathbf{x} - \mathbf{x}'|} \exp[-Q|\mathbf{x} - \mathbf{x}'|]. \quad (2.4)$$

When u is a parameter for preserving a dimension of a potential and l , Q^{-1} are the Gaussian and Coulomb screening lengths. We shall assume further that the doping concentration is very large ($n \rightarrow \infty$) and the potential is weak ($v \rightarrow 0$) so that nv^2 is finite.

A PATH-INTEGRAL FORMALISM

About fifty years ago, Feynman (1948) invented a new formulation for quantum mechanics called path integrals. This formalism was motivated by the paper of Dirac (1945) entitled "On The Analogy Between Classical and Quantum Mechanics". Rather than beginning with the Hamiltonian of a system, the Lagrangian is considered instead which allows us not involve to the commutation relations. The foundation concept is the amplitude, $\Phi[\mathbf{x}(\tau)]$, of a system moving along any path equal to the exponential of the phase of that path, where the phase is the ratio of the action, $S[\mathbf{x}(\tau)]$, along the path and Planck's constant. In notations

$$\Phi[\mathbf{x}(\tau)] = \exp\left[i \frac{S[\mathbf{x}(\tau)]}{\hbar}\right]. \quad (2.5)$$

Then we can define a propagator, which is an amplitude for a system going from one point to another point during a finite time, as a sum of $\Phi[\mathbf{x}(\tau)]$ over all possible paths. That is,

$$K(\mathbf{x}_2, \mathbf{x}_1; t, 0) = \sum_{\text{all possible paths}} \Phi[\mathbf{x}(\tau)], \quad (2.6)$$

where K is the propagator. Since the summation over all possible paths is not a precise mathematical definition, thus a path integral is introduced. For a propagator, we can write down its expression, using a path integral, as

$$K(\mathbf{x}_2, \mathbf{x}_1; t, 0) = \int D(\mathbf{x}(\tau)) \exp\left[\frac{i}{\hbar} S[\mathbf{x}(\tau)]\right]. \quad (2.7)$$

For more about path integrals, Feynman and Hibbs' book (1965) is the best one which gives us rather complete knowledge.

Now, we shall turn back to our problem. According to the last model, (2.4), the Lagrangian of our system is

$$L = \frac{1}{2}m\dot{x}^2 - \sum_{i=1}^N v(\mathbf{x} - \mathbf{x}'_i). \quad (2.8)$$

Using a path integral formalism, the propagator can be written as

$$K(\mathbf{x}_2, \mathbf{x}_1; t, 0; [\mathbf{x}']) = \int D(\mathbf{x}(\tau)) \exp\left[\frac{i}{\hbar} \int_0^t d\tau \left(\frac{1}{2}m\dot{x}^2 - \sum_{i=1}^N v(\mathbf{x} - \mathbf{x}'_i) \right)\right], \quad (2.9)$$

where $[\mathbf{x}']$ is a set of positions of impurities. From this propagator, the system properties obviously depend on a configuration of impurities which is random. But in practice we measure these quantities many times on the identical prepared system. It should be the average value, instead of the particular one, that will be obtained from the measurements. Kohn and Luttinger (1957) have shown that in general we can substitute the specific value of any function by its ensemble average provided that the impurities are truly independent.

Follow the foregoing discussion, we shall define the average propagator $\bar{K}(\mathbf{x}_2, \mathbf{x}_1; t, 0)$ as the sum over all configurations of the specific propagator $K(\mathbf{x}_2, \mathbf{x}_1; t, 0; [\mathbf{x}'])$ weighted with the probability $P([\mathbf{x}'])$ that the system having the configuration $[\mathbf{x}']$. The average propagator can be expressed mathematically by

$$\bar{K}(\mathbf{x}_2, \mathbf{x}_1; t, 0) = \sum_{\text{all configurations}} P([\mathbf{x}']) K(\mathbf{x}_2, \mathbf{x}_1; t, 0; [\mathbf{x}']), \quad (2.10)$$

where $K(\mathbf{x}_2, \mathbf{x}_1; t, 0; [\mathbf{x}'])$ is given by (2.9). Suppose that the impurities are completely random or uniformly distributed, we have

$$P([\mathbf{x}']) d[\mathbf{x}'] = \frac{1}{V^N} dx'_1 \cdots dx'_N, \quad (2.11)$$

where V is the volume of a semiconductor. Consequently,

$$\bar{K}(\mathbf{x}_1, \mathbf{x}_2; t, 0) = \int D(\mathbf{x}(\tau)) \exp\left[\frac{i}{\hbar} \int_0^t d\tau \frac{1}{2} m \dot{\mathbf{x}}^2\right] \left\{ \int \frac{d\mathbf{x}'}{V} \exp\left[-\frac{i}{\hbar} \int_0^t d\tau v(\mathbf{x} - \mathbf{x}')\right] \right\}^N. \quad (2.12)$$

Now, consider the term inside the curly braces of (2.12), putting in a new form, as

$$\int \frac{d\mathbf{x}'}{V} \exp\left[-\frac{i}{\hbar} \int_0^t d\tau v(\mathbf{x} - \mathbf{x}')\right] = 1 + \int \frac{d\mathbf{x}'}{V} \left(\exp\left[-\frac{i}{\hbar} \int_0^t d\tau v(\mathbf{x} - \mathbf{x}')\right] - 1 \right). \quad (2.13)$$

Applying the identity,

$$\lim_{V \rightarrow \infty} \left\{ 1 + \frac{a}{V} \right\}^N = \exp\left[\frac{aN}{V}\right], \quad (2.14)$$

and (2.13) into the last term of (2.12), this is reduced to

$$\left\{ \int \frac{dx'}{V} \exp \left[-\frac{i}{\hbar} \int_0^t d\tau v(\mathbf{x} - \mathbf{x}') \right] \right\}^N = \exp \left[n \int dx' \left(\exp \left[-\frac{i}{\hbar} \int_0^t d\tau v(\mathbf{x} - \mathbf{x}') \right] - 1 \right) \right], \quad (2.15)$$

where $n = \frac{N}{V}$ is the impurity concentration. Then expanding the exponential exponent in Taylor series, since $n \rightarrow \infty$, $v \rightarrow 0$ so that nv^2 is finite, we keep up terms to the second power of $v(\mathbf{x} - \mathbf{x}')$. The average propagator (2.12) becomes

$$\begin{aligned} \bar{K}(\mathbf{x}_2, \mathbf{x}_1; t, 0) = \int D(\mathbf{x}(\tau)) \exp \left[\frac{i}{\hbar} \left(\int_0^t d\tau \frac{1}{2} m \dot{\mathbf{x}}^2 - n \int_0^t d\tau \int dx' v(\mathbf{x} - \mathbf{x}') \right. \right. \\ \left. \left. + \frac{i}{2\hbar} n \int_0^t d\tau \int_0^t d\sigma \int dx' v(\mathbf{x}(\tau) - \mathbf{x}') v(\mathbf{x}(\sigma) - \mathbf{x}') \right) \right], \quad (2.16) \end{aligned}$$

Note that the assumption we used above allows us completely describe the system by the first and second moments of the potential. That is, the distribution of a potential is the Gaussian or normal distribution. This means that a system of an electron moving in weak and dense impurities is equivalent to moving in the Gaussian random potential.

We shall define the average potential energy \bar{V} and the autocorrelation function $W(\mathbf{x}(\tau) - \mathbf{x}(\sigma))$ as following:

$$\bar{V} = \int dx' v(\mathbf{x} - \mathbf{x}'), \quad (2.17)$$

and

$$W(\mathbf{x}(\tau) - \mathbf{x}(\sigma)) = \int d\mathbf{x}' v(\mathbf{x}(\tau) - \mathbf{x}') v(\mathbf{x}(\sigma) - \mathbf{x}') , \quad (2.18)$$

The autocorrelation function is an important function which tells us the effect of a potential at one point on a potential at another point. If the potential at any two points are uncorrelated then we shall call the Gaussian-white-noise random potential. The autocorrelation function of this potential is given by

$$W(\mathbf{x}(\tau) - \mathbf{x}(\sigma)) = D \delta(\mathbf{x}(\tau) - \mathbf{x}(\sigma)), \quad (2.19)$$

where D is a constant. By using these two functions, the average propagator can be written as

$$\bar{K}(\mathbf{x}_2, \mathbf{x}_1; t, 0) = \int D(\mathbf{x}(\tau)) \exp\left[\frac{i}{\hbar} \bar{S}[\mathbf{x}(\tau)]\right], \quad (2.20)$$

where

$$\bar{S}[\mathbf{x}(\tau)] = \int_0^t d\tau \left[\frac{1}{2} m \dot{\mathbf{x}}^2 - n \bar{V} + \frac{i}{\hbar} n \int_0^t d\sigma W(\mathbf{x}(\tau) - \mathbf{x}(\sigma)) \right]. \quad (2.21)$$

This trial action is sometimes called “two-time” trial action. It seems that the system can be viewed as an electron moving in the average potential with a “memory” effect. For two cases of potentials in which we are interested, the autocorrelation functions have the forms

$$W(\mathbf{x}(\tau) - \mathbf{x}(\sigma)) = u^2 (\pi L^2)^{-N} \exp\left[-\frac{|\mathbf{x}(\tau) - \mathbf{x}(\sigma)|}{L^2}\right], \quad (2.22)$$

and

$$W(\mathbf{x}(\tau) - \mathbf{x}(\sigma)) = \frac{2\pi Z^2 e^4}{\epsilon_0^2 Q} \exp[-Q|\mathbf{x}(\tau) - \mathbf{x}(\sigma)|], \quad (2.23)$$

for the Gaussian and screened Coulomb cases, respectively. When L is the new Gaussian screening length, $L^2 = 2l^2$.

THE DENSITY OF STATES

The density of states $\rho(E)$ (see Omar, 1975) can be defined by

$$\rho(E) dE = \text{a number of states between an energy interval } E \text{ and } E+dE \\ \text{per unit volume.} \quad (2.24)$$

This definition gives us a qualitative picture of the density of states, but does not explicitly express the formula for calculation. The usual formula for the density of states is concerned with the number-of-state function $N(E)$, which provides a number of states having an energy less than or equal to E ,

$$\rho(E) = \frac{dN(E)}{dE}. \quad (2.25)$$

Another formula which is directly related to the energy eigenvalue E_i of the eigenstate φ_i can be written as

$$\rho(E) = \frac{1}{V} \sum_i \delta(E - E_i), \quad (2.26)$$

where δ is the Dirac delta function.

In our work, it is easy to use the formula (2.26) since the Dirac delta function can be expressed in terms of the transformed propagator. With the energy expansion formula of the propagator (Feynman and Hibbs, 1965; Sakurai, 1985),

$$K(\mathbf{x}_2, \mathbf{x}_1; t, 0) = \sum_i \varphi_i(\mathbf{x}_2) \varphi_i^*(\mathbf{x}_1) \exp\left[-\frac{iE_i t}{\hbar}\right], \quad (2.27)$$

we have

$$\text{Tr} K(\mathbf{x}_2, \mathbf{x}_1; t, 0) = \sum_i \exp\left[-\frac{iE_i t}{\hbar}\right], \quad (2.28)$$

where Tr denotes the trace. Then taking a Fourier transform of both sides of (2.28), the result is

$$\int_{-\infty}^{\infty} dt \text{Tr} K(\mathbf{x}_2, \mathbf{x}_1; t, 0) \exp\left[\frac{iEt}{\hbar}\right] = 2\pi\hbar \sum_i \delta(E - E_i). \quad (2.29)$$

Note that the identities,

$$\delta(a) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp[iax] dx \quad (2.30)$$

and

$$\delta\left(\frac{a}{b}\right) = b\delta(a), \quad (2.31)$$

is used in the derivation of (2.29). Now the required relation between the density of states and the propagator is obtained by comparing (2.26) and (2.29), we have

$$\rho(E) = \frac{1}{2\pi\hbar} \frac{1}{V} \int_{-\infty}^{\infty} dt \text{Tr} K(\mathbf{x}_2, \mathbf{x}_1; t, 0) \exp\left[\frac{iEt}{\hbar}\right]. \quad (2.32)$$

For the heavily doped semiconductor, as already regarded, the propagator in (2.32) must be the average propagator (2.20) instead. That is, the density of states of our problem has a following form,

$$\rho(E) = \frac{1}{2\pi\hbar} \frac{1}{V} \int_{-\infty}^{\infty} dt \text{Tr} \bar{K}(\mathbf{x}_2, \mathbf{x}_1; t, 0) \exp\left[\frac{iEt}{\hbar}\right]. \quad (2.33)$$

From (2.32), it can be concluded that, in general, the density of states depends on the volume of a system. This dependence will be absent in certain systems. Such a system has the property

$$K(\mathbf{x}_2, \mathbf{x}_1; t, 0) = K(\mathbf{x}_2 - \mathbf{x}_1; t, 0), \quad (2.34)$$

which is the translational symmetry. The density of states (2.32) then becomes

$$\rho(E) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt K(\mathbf{x}_2, \mathbf{x}_2; t, 0) \exp\left[\frac{iEt}{\hbar}\right]. \quad (2.35)$$

For our propagator, we shall find that it satisfies the property (2.34) since we have averaged it over all configurations.