Chapter 5

Discussions and Conclusions

In this thesis, heavily doped strongly compensated semiconductor are studied by using the Feyman path integral method [8]. To be more specific, we calculate the density of states of HDCS [9,18,20,40] using the functional form proposed by Halperin and Lax [12]. The two parameters in the Halperin and Lax DOS are then computed by using the variational method based on the Feynman path integral.

Although the Halperin and Lax DOS agreed well with the experiments in the low energy band tail region and is a substantial improvement over Kane's [17] DOS, it has two limitations. Firstly, it requires numerical solution. Secondly, it cannot be extended to higher energies. For these reasons Sa-yakanit [26,27,28,29,30,31,32,33] developed a new theory based on the Feynman formulation of quantum mechanics. The Feynman formulation is useful since it expresses the electron propagation as a sum of classical-like paths. This is especially useful in disordered systems because the density of states can be calculated in much the

same way as in the Kane theory. Once the Feynman method is mastered, this is much simpler than the Schrödinger picture of quantum mechanics for disordered systems. The Feynman path integral approach was first applied to disordered systems by Edwards [5,6] and has subsequently been explored by others. However, Sa-yakanit succeeded in evaluating the path integrals explicitly and obtained an expression for DOS valid at all energies E. In the low energy limit the DOS reduces to a relatively simple analytic expression. At high energies, it reduces to that of the usual free electron. The path integral formulation begins with the full expression density of states [12]

$$\rho(E) = \frac{1}{V}\left\langle \sum_i \delta(E - E_i) \right\rangle, \tag{5.1}$$

here $\langle ... \rangle$ indicates an average over the ensemble of the scatterer position. Next the retarded propagator $K(\vec{x}_2, \vec{x}_1; t)$ is introduced to describe the propagation of an electron from point $\vec{x}_1$ to $\vec{x}_2$. The $\sum_i \delta(E - E_i)$ can be expressed in terms of the diagonal element ($\vec{x}_1 = \vec{x}_2$) of $K(\vec{x}_2, \vec{x}_1; t)$ giving

$$\rho(E) = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dt Tr K(\vec{x}_2, \vec{x}_1; t) \exp\left[\frac{iEt}{\hbar}\right]. \tag{5.2}$$

The average over $K(\vec{x}_2, \vec{x}_1; t)$ can be performed exactly as in the Kane theory by the equation

$$K(\vec{x}_2, \vec{x}_1; t,) = \int D[\vec{x}(\tau)] \exp\left(\frac{i}{\hbar} S\right), \tag{5.3}$$

where

$$S = \int_0^t d\tau \frac{m}{2}\dot{\vec{x}}^2(\tau) + \frac{i}{2\hbar}\int_0^t\int_0^t d\tau d\sigma W(\vec{x}(\tau) - \vec{x}(\sigma)). \tag{5.4}$$

Essentially the kinetic energy in S is included and typical fluctuation ξ_Q is replaced by $W(\vec{x}(\tau) - \vec{x}(\sigma))$, the autocorrelation of the potential energies. To proceed in calculating $K(\vec{x}_2, \vec{x}_1; t,)$, the full action S is modelled by a non-local harmonic "trial action" [25,40]

$$S_0(\omega) = \int_0^t d\tau \frac{m}{2}\dot{\vec{x}}^2(\tau) - \frac{m\omega^2}{4t}\int_0^t\int_0^t d\tau d\sigma[\vec{x}(\tau) - \vec{x}(\sigma)]^2. \tag{5.5}$$

From Eq. (5.3), we can write the average propagator as

$$K(\vec{x}_2, \vec{x}_1; t) = \int D[\vec{x}(\tau)] \exp[\frac{i}{\hbar}(S - S_0(\omega)) + \frac{i}{\hbar}S_0(\omega)]. \tag{5.6}$$

The full $K(\vec{x}_2, \vec{x}_1; t)$ can also be re-arranged as

$$K(\vec{x}_2, \vec{x}_1; t) = \int D[\vec{x}(\tau)] \exp[\frac{i}{\hbar}S_0(\omega)] \frac{\int D[\vec{x}(\tau)] \exp\{\frac{i}{\hbar}[S_0(\omega) + (S - S_0(\omega))]\}}{\int D[\vec{x}(\tau)] \exp[\frac{i}{\hbar}S_0(\omega)]}, \tag{5.7}$$

where

$$\langle O\rangle_{S_0(\omega)} = \frac{\int D[\vec{x}(\tau)] \exp[iS_0(\omega)/\hbar]O}{\int D[\vec{x}(\tau)] \exp[iS_0(\omega)/\hbar]}. \tag{5.8}$$

The average propagator is an exact expression but cannot be solved. The cumulant expansion,

$$\langle \exp[a]\rangle = \exp\left\{\langle a\rangle + \frac{1}{2!}[\langle a^2\rangle - \langle a\rangle^2] - \frac{1}{3!}[\langle a^3\rangle - 3\langle a^2\rangle\langle a\rangle + 2\langle a\rangle^3] + ...\right\}, \tag{5.9}$$

to the first cumulant [21] allows us to obtain the approximate propagator,

$$K_1(\vec{x}_2,\vec{x}_1;t,\omega) = K_0(\vec{x}_2,\vec{x}_1;t,\omega)\exp[\frac{i}{\hbar}\langle S - S_0(\omega)\rangle_{S_0(\omega)}]. \tag{5.10}$$

We can follow the detailed calculation of the density of states in Eq. (4.58). Finally, we find that the density of states deep in the tail with the first cumulant approximation in three dimensions can be expressed analytically for a screened Coulomb potential [12,25],

$$\rho(E) = \left[(E_Q Q)^3 a(\upsilon,z)/\xi_Q^2\right]\exp\left[-E_Q^2 b(\upsilon,z)/2\xi_Q\right], \tag{5.11}$$

where

$$a(\upsilon,z) = \frac{\left(\frac{3}{2}z^{-2}+\upsilon\right)^{3/2}}{4\sqrt{2}\pi^2 z^6\exp(z^2)\left[1-D_{-3}(z')\right]^2}, \tag{5.12}$$

and

$$b(\upsilon,z) = \frac{\left(\frac{3}{2}z^{-2}+\upsilon\right)^{2}}{2\exp\left(\frac{1}{2}z^2\right)\left[1-D_{-3}(z')\right]}. \tag{5.13}$$

Our density of states is dependent on the dimensionless parameters υ and z respectively. However, Halperin and Lax [12] have shown that the density of states depends only on the parameter υ. In the previous chapter, we have the relation between z and υ in Eq. (4.87). Then by substituting Eq. (4.86) into Eq. (5.12) and Eq. (5.13), the z-dependent of $a(\upsilon,z)$ and $b(\upsilon,z)$ can be eliminated but the obtained results are very complicated function. Nevertheless, our results can be shown analytically. The numerical values of $a(\upsilon)$ and $b(\upsilon)$ calculated

from eqs. (5.12) and (5.13) are given in Table 4.4. We also plot $a(v)$ and $b(v)$ as a function of v in Figure 5.1.

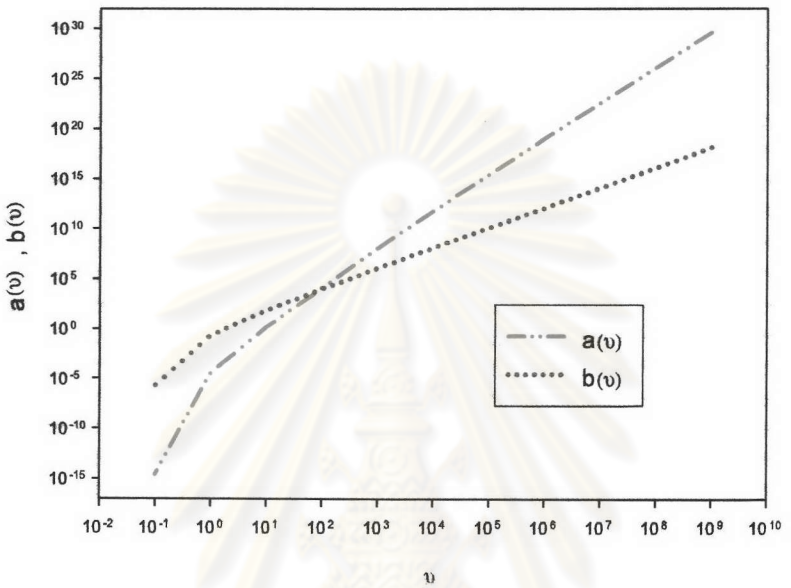

Figure 5.1 Plot of the preexponential $a(v)$ and the exponent $b(v)$ versus dimensionless energy v. Other important quantities of our interest are the logarithmic

derivative of the exponent $b(v,z)$ in Eq. (4.82) and the kinetic energy of localization $T(v,z)$ [12,26]. Both quantities can be expressed analytically as

$$n(v,z) = \frac{2v}{\left(\frac{3}{2}z^{-2} + v\right)}, \tag{5.14}$$

and

$$T(v,z) = \frac{3}{2}z^{-2}. \tag{5.15}$$

However, we can calculate the quantities $n(v)$ and $T(v)$ by substituting the parameter z (a function of v) in Eqs. (5.14) and (5.15). We also plot the logarithmic derivative of the exponent $n(v)$ versus the dimensionless energy v as shown in Figure 5.2. The critical exponent $n(v)$ has a value between 1 and 2. The ratio of the kinetic energy to the binding energy versus the dimensionless energy v is shown in Figure 5.3.

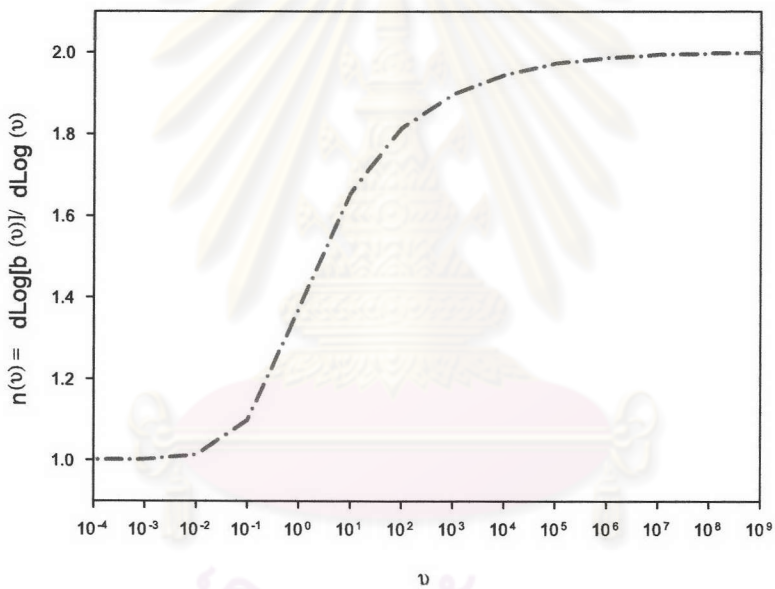

Figure 5.2 Plot of logarithmic derivative $n(v) = d\ln b(v)/d\ln v$ of the exponent $b(v)$ versus the dimensionless energy v.

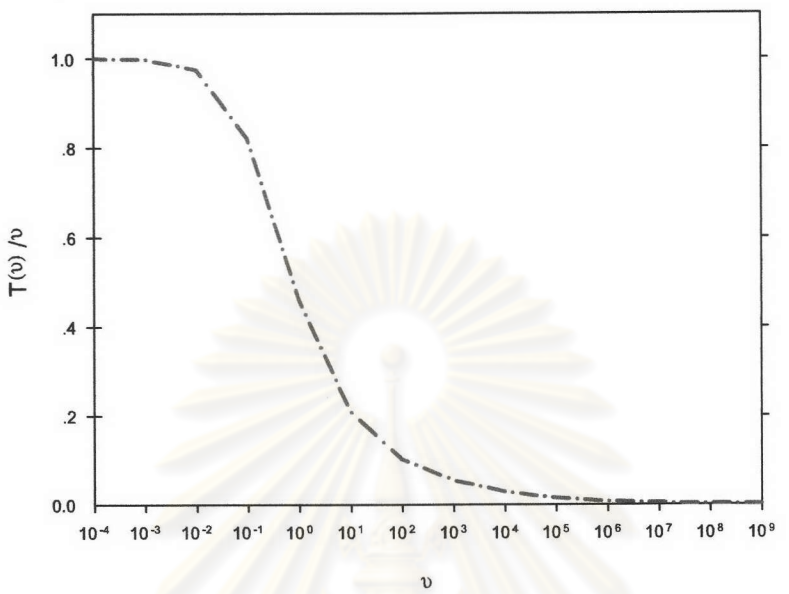

Figure 5.3 Plot of the ratio of the kinetic energy to the binding energy $T(v)/v$ versus the dimensionless energy v.

The calculated density of states near the tail of energy bands is very similar to the Urbach tail. The critical exponent n of our system has values between 1 and 2. This finding does not agree with $n = 2$ in the Kane theory. However, one knows that n must depend on the concentration of doping while in the Kane theory, n is a constant. Additionally, the density of states calculated by using the Kane theory is too large compared to the experimental value. The most important reason why the Kane theory cannot predict a correct DOS is that it neglects the zero point energy.

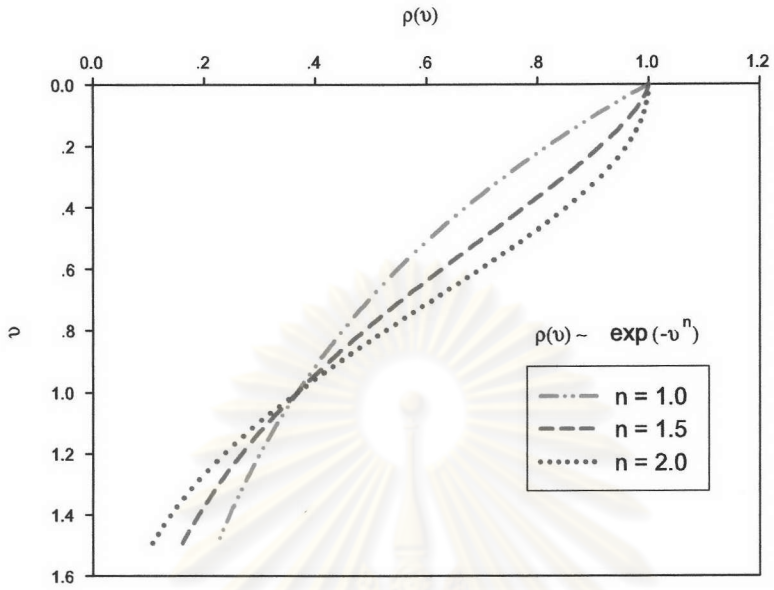

Figure 5.4 Density of states in the tail of HDCS GaAs.

The Feynman path integral method presented in this thesis is used to calculate the density of states in the energy band tail within the gap of heavily doped strongly compensated semiconductor for the screened Coulomb potential. Our work is similar to the theoretical studies of heavily doped semiconductor proposed by Sa-yakanit [30]. Theoretically, the studies of HDCS can give us a better understanding of disordered materials which have been used in advanced technology for decades. The aim of the thesis is also to gain some experience and familiarity with how to solve the problem in HDCS by the Feynman path integral method. It may be the basis for further study.