



THE CALCULATION OF BAND TAILS IN HEAVILY DOPED SEMICONDUCTORS

2.1 General Procedure¹.

In the presence of the random distribution of impurities in doped semiconductors, the data obtained in a macroscopic experiment come out as a result of the averaging over the random field configuration. Since the potential energy being randomly different in different parts of the sample. This fact is taken account of if the observable quantity, for instance, density of states, is calculated over the volume of a sample or of some big enough part which all the potential configurations available are expected to be met. In general, the calculation uses some particular form of potential energy V first, and then averages the result over the random configurations of potential energy V . To this end, the distribution function, $P[V]$, of the potential energy V will be defined. Both the form of $P[V]$ and the type of function V are defined according to a requirement of a problem. The existence of this distribution function $P[V]$ of a system of N random particles in volume Ω depends on the ... statistical conditions of probability theory that

$$N \longrightarrow \infty, \text{ and } \Omega \longrightarrow \infty,$$

but $0 < N/\Omega < \infty$.

2.2 Semiclassical Approach.

Kane⁷ used a semiclassical or Thomas - Fermi approximation to

calculate the density of states in each small region of doped semiconductors. The local density of states was assumed to be proportional to $\sqrt{(E - V)}$, where V was the local potential. For this approximation Kane assumed that the potential was sufficiently slowly varying that the potential energy could be treated as constant value over each region. The calculation of the average density of states then reduced to the determination of the distribution function for the potential of each region. In this section we will derive the Kane's density of states by using the physically intuitive idea of Kane but in different mathematical formulation.

If the small regions in doped semiconductors are large enough and the potential is sufficiently slowly varying, by using Thomas-Fermi method, the local density of states per unit volume of each region can be expressed as

$$\rho_{\ell}(E) = \frac{m^{*3/2}}{\sqrt{2} \pi^2 \hbar^2} \sqrt{E - V} H(E - V) \quad 2.2.1$$

which appropriate to a large volume. The Heaviside step function $H(x - \xi)$ is defined as

$$H(x - \xi) = \begin{cases} 1 & ; x > \xi \\ 0 & ; x < \xi \end{cases}$$

Because of the randomness of impurity distribution, the average values of potential energy in each region are random. So that, to obtain the total density of states, we must average this local density of states over all the values of V .

$$\rho_K(E) = \langle \rho_{\ell}(E) \rangle_V, \quad 2.2.2$$

where V is random variable.

The next stage is to determine the distribution function of V . Since the local potential is slowly varying, the average potential energy V can be approximated by the potential energy of electron in the field of all impurity potentials at centre of the considered region.

$$V = V(\vec{r}) = \sum_{i=1}^N v(\vec{r} - \vec{R}_i),$$

where $v(\vec{r} - \vec{R}_i)$ is potential energy of electron at point \vec{r} with respect to the i^{th} impurity atom at the position \vec{R}_i . Note that there are N impurity atoms over all the sample. By this approximation the distribution function $P[V]$ can be written in this form,

$$P[V] = \iiint \dots \int \frac{d\vec{R}_1}{\Omega} \frac{d\vec{R}_2}{\Omega} \dots \frac{d\vec{R}_N}{\Omega} \delta(V - \sum_{i=1}^N v(\vec{r} - \vec{R}_i)). \quad 2.2.3$$

The integral are all integrate over all volum Ω of the sample. Hence (2.2.2) can be rewritten in terms of $P[V]$ as follow

$$\rho(E) = \frac{m^*}{2^{1/2} \pi^{2/3} h^3} \int_{-\infty}^E P[V] \sqrt{E - V} dV. \quad 2.2.4$$

Now consider (2.2.3), the quantity $\frac{d\vec{R}_1}{\Omega} \frac{d\vec{R}_2}{\Omega} \dots \frac{d\vec{R}_N}{\Omega}$ is the probability that \vec{R}_1 is in the volume $d\vec{R}_1$, \vec{R}_2 is in the volume $d\vec{R}_2$...etc (since impurities are treated as complete random.) The Dirac delta function tells us that the configurations of these impurities are accepted if and only if $V = \sum_{i=1}^N v(\vec{r} - \vec{R}_i)$. So that, for simplicity, (2.2.3) can be written as

$$P[V] = \langle \delta(V - \sum_{i=1}^N v(\vec{r} - \vec{R}_i)) \rangle_{\{\vec{R}_i\}}. \quad 2.2.5$$

To evaluate (2.2.5), for convenience we transform Dirac delta function by Fourier integral and obtain

$$\delta(V - \sum_{i=1}^N v(\vec{r} - \vec{R}_i)) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(i\alpha \{ V - \sum_{i=1}^N v(\vec{r} - \vec{R}_i) \}) d\alpha .$$

Then on substituting this into (2.2.5) we get

$$P[V] = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\alpha \exp(i\alpha V) \langle \exp(-i\alpha \sum_{i=1}^N v(\vec{r} - \vec{R}_i)) \rangle_{\{\vec{R}_i\}} . \quad 2.2.6$$

If random variable \vec{R}_i are all independent the average term can be reduced to a simple form like this

$$\langle \exp(-i\alpha \sum_{i=1}^N v(\vec{r} - \vec{R}_i)) \rangle_{\{\vec{R}_i\}} = \langle \exp(-i\alpha v(\vec{r} - \vec{R})) \rangle_{\vec{R}}^N . \quad 2.2.7$$

The right hand side of (2.2.7) can be approximated by using cumulant expansion¹⁰. In this case only two order, first and second cumulant, are kept, and then the average in the right hand side of (2.2.7) can be approximated as

$$\begin{aligned} \langle \exp(-i\alpha v(\vec{r} - \vec{R})) \rangle &\approx \exp(-i\alpha \langle v(\vec{r} - \vec{R}) \rangle_{\vec{R}} \\ &\quad - \frac{\alpha^2}{2} \{ \langle v^2(\vec{r} - \vec{R}) \rangle_{\vec{R}} - \langle v(\vec{r} - \vec{R}) \rangle_{\vec{R}}^2 \}) \\ &= \exp\left(\frac{-i\alpha}{\Omega} \int v(\vec{r}-\vec{R}) d\vec{R} - \frac{\alpha^2}{2\Omega} \left\{ \int v^2(\vec{r}-\vec{R}) d\vec{R} - \right. \right. \\ &\quad \left. \left. - \frac{1}{\Omega} \left(\int v(\vec{r}-\vec{R}) d\vec{R} \right)^2 \right\} \right) . \end{aligned}$$

Since the assumption that the volume Ω must be large as introduced in the first section, then the last term can be dropped out and the equation (2.2.7) becomes

$$\langle \exp(-i\alpha \sum_{i=1}^N v(\vec{r}-\vec{R}_i)) \rangle_{\{\vec{R}_i\}} = \exp\left(\frac{N}{\Omega} \left\{ -i\alpha \int v(\vec{r}-\vec{R}) d\vec{R} - \frac{\alpha^2}{2} \int v^2(\vec{r}-\vec{R}) d\vec{R} \right\}\right) \quad 2.2.8$$

Placing this equation in (2.2.6), $P[V]$ becomes

$$P[V] = \frac{1}{2\pi} \int_{-\infty}^{\infty} da \exp(-i\alpha\{V+\bar{N} \int v(\vec{r}-\vec{R}) d\vec{R} - \frac{\alpha^2 \bar{N}}{2} \int v^2(\vec{r}-\vec{R}) d\vec{R}\}), \quad 2.2.9$$

where $\bar{N} = N/\Omega$.

As mention in Chapter I. Kane used the screened Coulomb potential to describe the potential of each impurity, the explicit form of this potential is

$$v(\vec{r} - \vec{R}) = -\frac{e^2}{\epsilon|\vec{r}-\vec{R}|} \exp(-Q|\vec{r}-\vec{R}|), \quad 2.2.10$$

and then the final form of $P[V]$ is

$$P[V] = \frac{1}{\sqrt{\pi\eta}} \exp(-(V-V_0)^2/\eta^2), \quad 2.2.11$$

where

$$V_0 = -4\pi e^2 \bar{N} / \epsilon Q^2,$$

$$\eta = e^2 (4\pi \bar{N} / Q)^{1/2} / \epsilon.$$

By substituting (2.2.10) into (2.2.4), the density of states becomes a function of E only as

$$\rho_K(E) = \frac{m^*3/2}{\sqrt{2\pi} \pi^2 N^3} \frac{1}{\eta} \int_{-\infty}^E \exp(-(V-V_0)^2/\eta^2) \sqrt{E-V} dV.$$

The integration part of this equation can be evaluated in terms of parabolic cylinder function^{11,12}

$$\rho_K(E) \approx \frac{m^*}{4\pi^2} \frac{\sqrt{\eta}}{\hbar^3} \frac{3/2}{2^{1/4}} \exp(-x^2/2) D_{-3/2}(-\sqrt{2} x), \quad 2.2.12$$

where $x = (E - V_0)/\eta$ and

$$D_\nu(Z) = \frac{\exp(-Z^2/4)}{\Gamma(-\nu)} \int_0^\infty t^{-\nu-1} \exp(Zt - t^2/2) dt. \quad 2.2.13$$

To consider the density of states at very high energy above V_0 and very low energy below V_0 , we use the asymptotic form of parabolic cylinder function¹² stating that ;

For $x \gg |v|$

$$D_\nu(x) \approx x \exp(-x^2/4), \quad 2.2.14$$

and $D_\nu(-x) \approx \frac{2}{\Gamma(-\nu)} x^{-\nu-1} \exp(x^2/4).$ 2.2.15

For $E \gg V_0$, we use (2.2.15) in (2.2.12), then obtain

$$\rho_K(E) \approx \frac{m^*}{2\pi^2 \hbar^3} \sqrt{E - V_0} \quad ; \quad E \gg V_0. \quad 2.2.16$$

This equation is equivalent to the result obtaining from free electron model.

When the deep tail states, $E \ll V_0$, are considered, the equation (2.2.14) is used instead of (2.2.15) and then the result shows tail of density of states

$$\rho_K(E) \approx \frac{m^*{}^{3/2} n (V_0 - E)^{-3/2}}{8\pi^2 \hbar^3} \exp(-(E - V_0)^2 / \eta^2); E \ll V_0. \quad 2.2.17$$

This expression shows that when the considered energy is below V_0 the density of states does not vanish. There is an exponential tail when E is very low.

Note that the tail of density of states derived by Kane is in a Gaussian form only. This result does not agree with the experiments⁸ because the experimental results show that density of states is proportional to $\exp(-|E|^n)$ where n is some number between 0.5 and 2.

Another unsatisfactory point is that the numerical values of density of states at deep tail are all larger than those observed and the length of the Gaussian tail is longer than the results from experiments.

The reason is that local density of states in each small region of sample is approximated by free electron model for large sample. For large sample this model treat that all eigenstates of an electron as being continuous and the lowest energy or zero point energy of electron is equal to the average potential energy of the sample. But, for a small region, the continuity of eigenstates does not occur and zero point energy is greater than the average potential energy V . But the semiclassical approximation assumes that the eigenstates in each small region is continuous. Therefore, the excess states, that do not occur in the discontinuous case, will be included in an averaging procedure using to calculate average density of states which produce over estimate values of density of states.

2.3 Wave Mechanics Method⁸

To reduce the large values of Kane's density of states, Halperin and Lax solved for the discrete eigenstates of the random potential by using trial wave function. Also they included the kinetic energy of localization (zero point energy), which was omitted in Kane's method, in their calculation. The idea behind their calculation will be discussed briefly in this section. A more details of calculation can be found in the reference⁸.

The simplest approximation in the high density impurities is that the electron is treated moving in an uniform potential energy equal to the average potential energy of all impurity atoms. The density of states in this approximation vanishes completely for energy below a minimum energy E_0 which is equal to the average value of impurity potentials. In the real sample, we know that the density of states does not vanish below the energy E_0 . Because of the random nature of the impurity distribution, there will be some macroscopic region of crystal in which we will find higher or lower densities than the average density. Hence the average potential energy of an electron in this region will be lower or greater than the average value of the sample as a whole. If the region in question is sufficiently large and the potential energy is sufficiently low, then we expect to find a bound state, localized in this region, with an energy less than E_0 .

The density of states is now calculated from the definition that

$$\rho(E) = \frac{1}{\Omega} \langle \sum_i \delta(E - E_i) \rangle_V \quad 2.3.1$$

where E_i is the energy of the i^{th} eigenstate of the Hamiltonian H , and Ω is the volume of the sample. For doped semiconductors, the Hamiltonian H of an electron carrier (or hole) is assumed to be

$$H = T + V(\vec{r}) \quad , \quad 2.3.2$$

where

$$T = -\frac{\hbar^2 \nabla^2}{2m^*} + E_0 \quad , \quad 2.3.3$$

and

$$V(\vec{r}) = \sum_{i=1}^N v(\vec{r} - \vec{R}_i) - E_0 \quad 2.3.4$$

$V(\vec{r})$ defined by (2.3.4) yield the result that its average value will be equal to zero. The quantity $v(\vec{r} - \vec{R}_i)$ is an impurity potential as described in section 2.2

To evaluate the eigenenergy E_i , the wavefunction $\psi_i(\vec{r})$ must be known first. But because of the complexity of the potential part in Hamiltonian H , it is very hard to find the exact form of this wave function. However, the variational principle ensures that an appropriate wavefunction, which gives an eigenenergy very close to the true value can be determined. The process begins by assuming an approximate trial wavefunction first and then the form of this trial wavefunction is adjusted until it approaches the most probable form determined by the variational condition.

At this stage, the behavior of wavefunction as it relates to local impurity densities should be known. In the high impurity density limit it is assumed that the range of a single impurity potential is small compared with the width of the wavefunction. For simplicity, attractive impurities

are considered only. If the wavefunction of energy $E \ll E_0$ is very spread out, its kinetic energy of localization will be very small, and the necessary potential energy in this region of wavefunction will differ from the average potential energy in the sample by the amount $E - E_0$. The required excess density of impurities in this region must be such to give an average potential energy of $E - E_0$. On the other hand if the wavefunction is assumed to be very narrow, then the kinetic energy of localization will be very large. Consequently the excess density of impurities required in this region of wavefunction must be very high in order that the average of $V(\vec{r})$ in this region is negative below $E - E_0$.

Next, if the wavefunction is assumed to be too narrow, the probability of finding the required excess impurity density in the region of wavefunction becomes extremely small. Also, if the wavefunction is assumed to be too large, the probability of finding the high excess density of impurities in a large region becomes extremely small also. Now it can be seen that there will be a most probable shape for a wavefunction, not too narrow and not too spread out.

Let us assume that the wavefunction $\psi_1(\vec{r})$ is approximated by trial wavefunction $f(\vec{r} - \vec{r}_0)$,

$$\psi_1(\vec{r}) \approx f(\vec{r} - \vec{r}_0).$$

In this case $f(\vec{r} - \vec{r}_0)$ is a real value function satisfying the normalization condition

$$\int f^2(\vec{r} - \vec{r}_0) d\vec{r} = 1.$$

\vec{r}_0 is a position variable used to determine the position of function f at any point through out the sample. For the case of very low energy below E_0 , it can be assumed that the function f has the same shape at any position of \vec{r}_0 . From this assumption, an approximated average energy of electron at the point \vec{r}_0 is obtain as

$$E(\vec{r}_0) = \int f(\vec{r} - \vec{r}_0) Hf(\vec{r} - \vec{r}_0) d\vec{r} \quad 2.3.5$$

If H is given by equation (2.3.2), then equation (2.3.5) can be rewritten as

$$E(\vec{r}_0) = \theta + V_s(\vec{r}_0) \quad , \quad 2.3.6$$

where $\theta = \int f(\vec{r} - \vec{r}_0) T f(\vec{r} - \vec{r}_0) d\vec{r} \quad , \quad 2.3.7$

$$V_s(\vec{r}_0) = \int f^2(\vec{r} - \vec{r}_0) V(\vec{r}) d\vec{r} \quad . \quad 2.3.8$$

The potential energy $V_s(\vec{r}_0)$ is an average of the potential energy $V(\vec{r})$ in a region of f . As \vec{r}_0 is permitted to vary throughout the sample, $V_s(\vec{r}_0)$ will fluctuate about an average value of zero. In general, the energies of all physical systems have tendency to decrease to as small values as possible. Thus, it can be assumed that the best approximated eigenenergies $E_1(\vec{r}_0)$ obtained from trial wavefunction f are equal to the minimum values of the average energy function $E(\vec{r}_0)$, not necessarily the absolute minimum. Because the operator T is translationally invariant the kinetic term, θ , will be independent of \vec{r}_0 . Hence the behavior of $E(\vec{r}_0)$ will depend on $V_s(\vec{r}_0)$ only. Therefore the best approximated

eigenenergies can be determined by

$$E_i(\vec{r}_0) = E_i(\vec{y}_i) = \theta + V_s(\vec{y}_i),$$

where $\{\vec{y}_i\}$ is the set of all points satisfying

$$\vec{\nabla} V_s(\vec{y}_i) = 0,$$

and the second derivatives are positive at \vec{y}_i . Note that the variational principle indicates that the energies $E(\vec{y}_i)$ are all greater than the true values of eigenenergy E_i ,

$$E(\vec{y}_i) > E_i.$$

If there is a one-to-one correspondence between local minima in $E(\vec{r}_0)$ and the eigenenergies, then the number of eigenstates with energy E is approximately equal to the number of local minima in $E(\vec{r}_0)$ with value E . The approximate density of states in the volume Ω is defined by

$$\rho_f(E) = \frac{1}{\Omega} \langle \sum_i \delta(E - \theta - V_s(\vec{y}_i)) \rangle_{V_s},$$

or in a new form

$$\rho_f(E) = \frac{1}{\Omega} \int d\vec{y} \langle \sum_i \delta(\vec{y} - \vec{y}_i) \delta(E - \theta - V_s(\vec{y})) \rangle_{V_s}.$$

When the concentration of impurities is sufficiently high, the random variable $V_s(\vec{y})$ obeys Gaussian statistics. From this stage, Halperin and Lax were able to evaluate $\rho_f(E)$, for three dimension, and got

$$\rho_f(E) = \frac{\sigma_1 \sigma_2 \sigma_3 (\theta - E)^3}{(2\pi)^2 \xi^2 \sigma_0^7} \exp(-(\theta - E)^2 / 2\xi \sigma_0^2) . \quad 2.3.9$$

where ξ is a constant proportional to the concentration of impurities, \bar{N} . The quantities σ_0 , σ_1 , σ_2 and σ_3 are defined as follow ;

$$\sigma_0^2 = G(\vec{0}) \quad 2.3.10$$

and

$$\nabla \nabla G(\vec{y}) \Big|_{\vec{y} = \vec{0}} = - \begin{bmatrix} \sigma_1^2 & 0 & 0 \\ 0 & \sigma_2^2 & 0 \\ 0 & 0 & \sigma_3^2 \end{bmatrix} , \quad 2.3.11$$

where

$$G(\vec{y} - \vec{y}') = \iint f^2(\vec{x} - \vec{y}) f^2(\vec{x}' - \vec{y}') W(\vec{x} - \vec{x}') d\vec{x} d\vec{x}' . \quad 2.3.12$$

and

$$W(\vec{x} - \vec{x}') = \int v(\vec{x} - \vec{R}) v(\vec{x}' - \vec{R}) d\vec{R} . \quad 2.3.13$$

Now, Let us consider the problem of finding the best trial wavefunction f . We know that regardless of the choice of f , the variational estimates of the energies of the eigenstates will be higher than the true values. So that, in the low energy tail, any approximation which systematically over estimates the energies of all the eigenstates will underestimate the density of states. And hence in the low-energy tail, no matter what the choice of f , $\rho_f(E)$ will be smaller than the true density of states, $\rho(E)$. Clearly the best choice of f , for any given energy E , is that which maximizes $\rho_f(E)$. We have

$$\rho(E) = \max_f \{ \rho_f(E) \}$$

Halperin and Lax considered only the exponential part of (2.3.9). They treated the limit $\xi \rightarrow 0$ when the exponential factor is dominant. The best choice of f is that which maximizes the exponential factor in (2.3.9), or minimizes the quantity $\left[\frac{E - E_0}{\sigma_0} \right]^2$. To minimize this quantity Halperin and Lax looked at the solution of a nonlinear integral equation,

$$Tf(\vec{x}) - \mu f(\vec{x}) \int f^2(\vec{x}') W(\vec{x} - \vec{x}') d\vec{x}' = Ef(\vec{x}),$$

where μ is a Lagrange multiplier. By substituting the operator T given by (2.3.3), this equation becomes

$$\frac{\hbar^2 \nabla^2}{2m^*} f(\vec{x}) - \mu f(\vec{x}) \int f^2(\vec{x}') W(\vec{x} - \vec{x}') d\vec{x}' = (E - E_0) f(\vec{x}). \quad (2.3.14)$$

This equation looks like the Hartree equation for a particle bound in its own self-consistent field, with an interaction- $\mu W(\vec{x} - \vec{x}')$. The equation can be solved by computer using the techniques developed by Hartree.

For each value of $E - E_0$ a trial function $f(\vec{x})$ is first used to evaluate the quantity $\int f^2(\vec{x}') W(\vec{x} - \vec{x}') d\vec{x}'$ in the equation (2.3.14). Then the value of μ is varied until the solution $f(\vec{x})$ of (2.3.14) satisfies the required boundary conditions. Next, the function $f(\vec{x})$ thus obtained is used as a new trial function to evaluate the new value of the quantity $\int f^2(\vec{x}') W(\vec{x} - \vec{x}') d\vec{x}'$. Now the process reverts to the previous step to solve a new wavefunction $f(\vec{x})$. This iteration process will be carried on until the new wavefunction and the old one are approximately equal.

For screened Coulomb potential of impurities defined by (2.2.10) we obtain

$$W(\vec{x} - \vec{x}') = (\xi/\bar{N}) \exp(-Q|\vec{x} - \vec{x}'|)$$

where $\xi = 2\pi e^4 \bar{N}/Q\epsilon^2$

Because screened Coulomb potential has spherical symmetry the quantities σ_1 , σ_2 and σ_3 are all equal and have the value

$$\sigma_1 = 1/3 \bar{v}_{\vec{y}=\vec{c}}^2 G(\vec{y}).$$

If the dimensionless quantities are introduced, i.e.,

$$E_Q = \pi^2 Q^2 / 2m^*$$

and $v = (E_0 - E)/E_Q,$

then the density of states can be written in these new quantities as

$$\rho(E) = \left[\frac{E_Q^3 Q^3}{\xi^2} \right] \frac{\sigma_1^3 (T+v)^3}{(2\pi)^2 \sigma_c^7} \exp\left(-\frac{E_Q}{2\xi} \left\{ \frac{T+v}{\sigma_c} \right\}^2\right),$$

or

$$\rho(E) = (E_Q Q^3 / \xi^2) a(v) \exp(-E_Q^2 b(v) / 2\xi) \quad 2.3.25$$

$a(v)$ and $b(v)$ are dimensionless function.

Halperin and Lax considered only the ground state of the wavefunction $f(\vec{x})$ in the process of calculation. They obtained the numerical values of $a(v)$ and $b(v)$ listed in table 2.1

As we mention, the density of states obtained from experiments are of the form

$$\rho(E) \propto \exp(-|E|^n),$$

where $1/2 < n < 2$.

By their calculation, Halperin and Lax got the quantity n agree with the experiment. They were able to obtain the numerical values of n by using the equation

$$n = \frac{d(\ln b(v))}{d(\ln v)} \quad (2.3.16)$$

The graph of n plotted against the quantities v is shown in Fig. 2.1.

The values of the density of states are given for ξ' having the values 0.05, 0.5, 5 and 50 in Table 2.1 respectively. These values were calculated from equation

$$\rho(E) = a(v) \exp(-b(v)/2\xi') \quad (2.3.17)$$

where $\xi' = \xi/E_Q^2$.

This equation comes from the equation (2.3.15) by dropping out the constant factor E_Q^3/ξ^2 .

Since Halperin and Lax used only the ground state energies in their calculation, the values of density of states were an under estimate of the true values. This results from the fact that there may be some excited states in some regions having the same energies as the ground states energies in other ones. These excited states was neglected in the calculation. Hence the number of states at energy E should be reduced by amount of number of these excited states and consequently the density of

Table 2.1 Numerical values of $a(v)$, $b(v)$, and $\rho(v)$. The values of $a(v)$ and $b(v)$ are all calculated by Halperin and Lax.

v	$a(v)$	$b(v)$	$\rho(v)$			
			$\xi=50$	$\xi=5$	$\xi=0.5$	$\xi=0.05$
1.00×10^3	3.098×10^8	1.444×10^6	0.000	0.000	0.000	0.000
5.62×10^2	4.645×10^7	4.912×10^5	0.000	0.000	0.000	0.000
3.162×10^2	7.250×10^6	1.702×10^5	0.000	0.000	0.000	0.000
1.78×10^2	1.153×10^6	6.00×10^4	0.000	0.000	0.000	0.000
1.00×10^2	1.888×10^5	2.150×10^4	7.993×10^{-89}	0.000	0.000	0.000
5.62×10	3.223×10^4	7.808×10^3	3.968×10^{-30}	0.000	0.000	0.000
3.16×10	5.781×10^3	2.988×10^3	6.099×10^{-10}	0.000	0.000	0.000
1.78×10	1.094×10^3	1.167×10^3	9.350×10^{-3}	2.274×10^{-48}	0.000	0.000
1.00×10	2.197×10^2	4.716×10^2	1.967	7.253×10^{-19}	0.000	0.000
5.62	4.689×10	1.983×10^2	6.455	1.146×10^{-7}	3.552×10^{-85}	0.000
3.16	1.078×10	8.720×10	4.507	1.760×10^{-3}	1.453×10^{-37}	0.000
1.78	2.793	4.043×10	1.864	4.900×10^{-2}	7.719×10^{-18}	0.000
1.00	7.259×10^{-1}	1.956×10	5.969×10^{-1}	1.027×10^{-1}	2.323×10^{-9}	8.182×10^{-86}
5.62×10^{-1}	2.157×10^{-1}	1.008×10	1.950×10^{-1}	7.872×10^{-2}	9.048×10^{-6}	3.606×10^{-45}
3.16×10^{-1}	5.957×10^{-2}	5.456	5.641×10^{-2}	3.452×10^{-2}	2.544×10^{-4}	1.202×10^{-25}
1.78×10^{-1}	2.423×10^{-2}	3.108	2.349×10^{-2}	1.776×10^{-2}	1.083×10^{-3}	7.700×10^{-16}
1.00×10^{-1}	8.906×10^{-3}	1.846	8.743×10^{-3}	7.405×10^{-3}	1.406×10^{-3}	8.563×10^{-11}
5.62×10^{-2}	3.532×10^{-3}	1.151	3.492×10^{-3}	3.148×10^{-3}	1.117×10^{-3}	3.542×10^{-8}
3.16×10^{-2}	1.485×10^{-3}	7.516×10^{-1}	1.474×10^{-3}	1.377×10^{-3}	7.003×10^{-4}	8.083×10^{-7}
1.78×10^{-2}	5.407×10^{-4}	5.006×10^{-1}	5.380×10^{-4}	5.143×10^{-4}	3.278×10^{-4}	3.621×10^{-6}
1.00×10^{-2}	2.834×10^{-4}	3.43×10^{-1}	2.824×10^{-4}	2.738×10^{-4}	2.011×10^{-4}	9.178×10^{-6}

states at this energy E are lower than the true values.

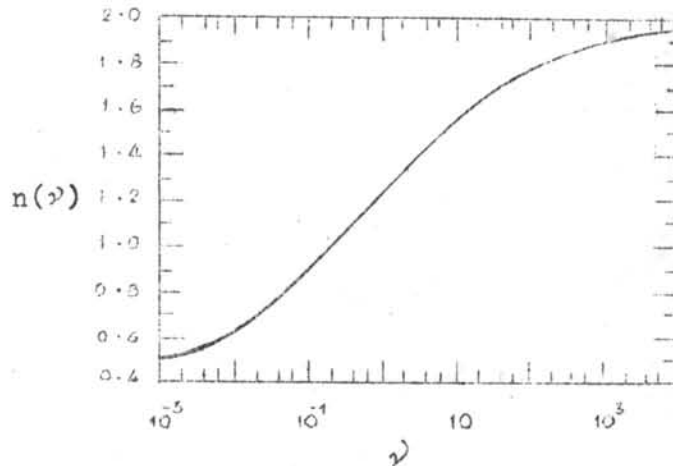


Fig. 2.1 The logarithmic derivative $n = [d \ln b(v)] / [d \ln v]$ of the exponent $b(v)$ in the density of states is shown to vary smoothly from $n = 1/2$ to 2.

2.4 Path Integral Approach.^{9,13-20}

Sa-yakanit^{9,17} has introduced another method for calculating the density of states in heavily doped semiconductors. It is Feynman Path Integration technique. The density of states evaluated by this method agrees with that evaluated by Halperin and Lax, i.e.,

$$\rho(E) = (A(E)/\xi^2) \exp(-E(E)/2\xi).$$

The functions $A(E)$ and $B(E)$ evaluated by path integral method are expressed analytically in terms of parabolic cylinder function. Although, it is more difficult to obtain the numerical values of parabolic cylinder function than from the evaluation of ordinary algebraic cylinder function, it is more convenient to calculate the density of states by evaluating parabolic cylinder function than by solving Hartree's equation as was done by Halperin and Lax. To find the appropriate values of density of states using path integration method, we only have to find the root of an equation of parabolic cylinder function. The outline of path integration method is as follow.

We begin with the density of states as defined by (2.3.1),

$$\rho(E) = \frac{1}{\Omega} \langle \sum_i \delta(E - E_i) \rangle_V .$$

This equation can be expressed in terms of the propagator (Green's function) for a single electron moving in the field of N impurities as

$$\begin{aligned} \rho(E) &= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \exp(iEt/\hbar) \langle \mathcal{G}(0,0;t,\{v\}) \rangle_V \\ &= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt G(0,0;t) \exp(iEt/\hbar) \end{aligned} \quad 2.4.1$$

where $G(\vec{r}_2, \vec{r}_1; t)$ is the average propagator in the random potential of all impurities. The propagator $\mathcal{G}(\vec{r}_2, \vec{r}_1; t, \{v\})$ satisfies the equation¹⁸

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

which can be expressed in the path integral representation as

$$\mathcal{G}(\vec{r}_2, \vec{r}_1; t, \{v\}) = \int \mathcal{D}(\vec{r}(\tau)) \exp\left(\frac{i}{\hbar} \int_0^t d\tau \left\{ \frac{m^* \dot{\vec{r}}^2(\tau)}{2} - \sum_i v(\vec{r}(\tau) - \vec{R}_i) \right\}\right). \quad 2.4.2$$

where $v(\vec{r} - \vec{R}_i)$ is the i^{th} impurity potential energy. Notation $\mathcal{D}(\vec{r}(\tau))$ denotes the path integral to be carried out with the boundary conditions $\vec{r}(0) = \vec{r}_1$ and $\vec{r}(t) = \vec{r}_2$. Note that the operator H is defined

$$\text{as} \quad H(\{v\}) = - \frac{\hbar^2 \nabla^2}{2m^*} + \sum_i v(\vec{r} - \vec{R}_i).$$

By assuming that the impurity potential V is weak but that their density \bar{N} is high so that $\bar{N}v^2$ is finite we find that the average propagator can be expressed in the form

$$\langle \mathcal{G}(\vec{r}_2, \vec{r}_1; t, \{v\}) \rangle_V = G(\vec{r}_2, \vec{r}_1; t) = \int \mathcal{D}(\vec{r}(\tau)) \exp(iS/\hbar) \quad 2.4.3$$

where S is the action of the random system given as

$$S = \int_0^t d\tau \left\{ \frac{m^* \dot{\vec{r}}^2(\tau)}{2} - E_0 + \frac{i}{2\hbar} \bar{N} \int_0^t d\sigma W(\vec{r}(\tau) - \vec{r}(\sigma)) \right\}, \quad 2.4.4$$

and W is defined by (2.3.13), E_0 is the average of potential energy of electron over all the impurities potential

$$E_0 = \int d\vec{R} v(\vec{r} - \vec{R}).$$

For an impurity potential of the screened Coulomb form given by (2.2.10) the function $W(\vec{r}(\tau) - \vec{r}(\sigma))$ becomes

$$W(\vec{r}(\tau) - \vec{r}(\sigma)) = (\xi/\bar{N}) \exp(-Q|\vec{r}(\tau) - \vec{r}(\sigma)|), \quad 2.4.5$$

$$\text{and} \quad E_0 = -4\pi e^2/\epsilon Q^2 \quad 2.4.6$$

where $\xi = 2\pi e^4 \bar{N} / Q \epsilon^2$ has the dimension of the energy square.

The action associated with the above quantities is

$$S = \int_0^t d\tau \left\{ \frac{m^* \dot{\vec{r}}^2(\tau)}{2} - E_0 + \frac{i}{2\hbar} \xi \int_0^t d\sigma \exp(-Q |\dot{\vec{r}}(\tau) - \dot{\vec{r}}(\sigma)|) \right\} \quad 2.4.7$$

In general the path integral of this action is very difficult to evaluate analytically because it is not quadratic in $\dot{\vec{r}}$. To perform the path integral in (2.4.3), an action which is simple, integrable and similar to the action S in rough approximation must be assumed. This can be achieved by modelling the action S by S_0 ^{17,18},

$$S_0(\omega) = \int_0^t \frac{m^*}{2} d\tau \{ \dot{\vec{r}}^2(\tau) - \frac{\omega^2}{2t} \int_0^t d\sigma |\dot{\vec{r}}(\tau) - \dot{\vec{r}}(\sigma)|^2 \} \quad 2.4.8$$

where ω is a parameter to be determined later. Then we can rewrite the equation (2.4.3) in a new form

$$G(\vec{r}_2, \vec{r}_1; t) = G_0(\vec{r}_2, \vec{r}_1; t, \omega) \langle \exp(i(S - S_0(\omega))/\hbar) \rangle_{S_0(\omega)} \quad 2.4.9$$

where the propagator $G_0(\vec{r}_2, \vec{r}_1; t, \omega)$ is defined by

$$G_0(\vec{r}_2, \vec{r}_1; t, \omega) = \int \mathcal{D}(\dot{\vec{r}}(\tau)) \exp(i S_0(\omega)/\hbar) \quad 2.4.10$$

and the average $\langle \rangle_{S_0(\omega)}$ is defined as

$$\langle P \rangle_{S_0(\omega)} = \frac{\int \mathcal{D}(\dot{\vec{r}}(\tau)) \exp(i S_0(\omega)/\hbar) P}{\int \mathcal{D}(\dot{\vec{r}}(\tau)) \exp(i S_0(\omega)/\hbar)} \quad 2.4.11$$

Further, the equation (2.4.9) can be approximated by keeping only the first cumulant, i.e.,

$$G_1(\vec{r}_2, \vec{r}_1; t) = G_0(\vec{r}_2, \vec{r}_1; t, \omega) \exp((i/\hbar) \langle S - S_0(\omega) \rangle_{S_0(\omega)}) \quad 2.4.12$$

Note that $G_1(\vec{r}_2, \vec{r}_1; t)$ is defined as being the first cumulant approximation of $G(\vec{r}_2, \vec{r}_1; t)$.

To obtain the density of states we need only the diagonal part of the average propagator, $G_1(0, 0; t)$. Then equation (2.4.12) becomes

$$G_1(0, 0; t) = G_0(0, 0; t, \omega) \exp((i/\hbar) \langle S - S_0(\omega) \rangle_{S_0(\omega); \vec{r}_1 = \vec{r}_2 = \vec{0}}) \quad 2.4.13$$

The propagator $G_0(0, 0; t, \omega)$ can be evaluate exactly to yield the result

$$G_0(0, 0; t, \omega) = \left\{ \frac{m^*}{2\pi i \hbar t} \right\}^{3/2} \left\{ \frac{\omega t}{2 \sin \frac{\omega t}{2}} \right\}^3. \quad 2.4.14$$

The average $\langle S - S_0 \rangle_{S_0; \vec{r}_1 = \vec{r}_2 = \vec{0}}$ is given by⁹,

$$\begin{aligned} \langle S - S_0(\omega) \rangle_{S_0(\omega); \vec{r}_1 = \vec{r}_2 = \vec{0}} &= -\frac{3i\hbar}{2} \left(\frac{\omega t}{2} \cot \frac{\omega t}{2} - 1 \right) - E_0 t \\ &+ \frac{iQt\zeta}{2\hbar\sqrt{\pi}} \int_0^t dx \int_0^x dy y \exp(-Q^2 y) (j(y, x, \omega, t))^{-3/2}, \end{aligned} \quad 2.4.15$$

$$\text{where } j(y, x, \omega, t) = y + \frac{i\hbar}{m^*\omega} \left(\sin \frac{\omega x}{2} \sin \frac{\omega(t-x)}{2} / \sin \frac{\omega t}{2} \right). \quad 2.4.16$$

To obtain the approximated density of states we substitute (2.4.13), (2.4.14) and (2.4.15) into (2.4.1) and obtain

$$\rho_1(E, \omega) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \left(\frac{m^*}{2\pi i \hbar t} \right)^{3/2} \left(\frac{\omega t}{2 \sin \frac{\omega t}{2}} \right)^3 \exp\left(\frac{3}{2} \left(\frac{\omega t}{2} \cot \frac{\omega t}{2} - 1 \right) - \frac{i}{\hbar} (E_c - E) t\right) \\ - \frac{Qt\xi}{2\hbar^2 \sqrt{\pi}} \int_0^t dx \int_0^{\omega} dy y \exp(-Q^2 y) (j(y, x, \omega, t))^{-3/2} \quad (2.4.17)$$

If we let $x = t\zeta$, the above equation becomes

$$\rho_1(E, \omega) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \left(\frac{m^*}{2\pi i \hbar t} \right)^{3/2} \left(\frac{\omega t}{2 \sin \frac{\omega t}{2}} \right)^3 \exp\left(\frac{3}{2} \left(\frac{\omega t}{2} \cot \frac{\omega t}{2} - 1 \right) - \frac{i}{\hbar} (E_c - E) t\right) \\ - \frac{\xi Q t^2}{2\sqrt{\pi} \hbar^2} \int_0^1 d\zeta \int_0^{\omega} dy y \exp(-Q^2 y) (j(y, \zeta, \omega, t))^{-3/2} \quad (2.4.18)$$

$$\text{and } j(y, \zeta, \omega, t) = y + \frac{i\hbar}{\omega} \left(\sin \frac{\omega t \zeta}{2} \sin \frac{\omega t (1-\zeta)}{2} / \sin \frac{\omega t}{2} \right) \quad (2.4.19)$$

To obtain the density of states in tail region we consider the ground state contribution by letting $t \rightarrow \infty$. Then (2.4.18) becomes⁹

$$\rho_1(E, \omega) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \left(\frac{m^*}{2\pi i \hbar t} \right)^{3/2} (i\omega t)^3 \exp\left(-\frac{3i\omega t}{4} - \frac{i}{\hbar} (E_c - E) t\right) \\ - \frac{\sqrt{2} \xi t^2}{\sqrt{\pi} \hbar^2} \exp(Z^2/4) D_{-3}(Z), \quad (2.4.20)$$

$$\text{where}^{12} \quad \frac{\sqrt{2} \xi}{\sqrt{\pi} \hbar^2} \exp(Z^2/4) D_{-3}(Z) = \frac{\xi}{2\pi^2 \sqrt{\pi}} \int_0^{\infty} dy y \exp(-Q^2 y) \left(y + \frac{\hbar}{2m^* \omega} \right)^{-3/2}$$

$$\text{and } Z^2 = \hbar Q^2 / \omega m^* .$$

$D_p(Z)$ is parabolic cylinder function as defined by (2.2.13).

For convenience we change some quantities to new forms.

Let $E_Q = \hbar^2 Q^2 / 2m^*$, $E_\omega = \hbar\omega^2$ and $v = (E_0 - E) / E_Q$ then $Z^2 = 2E_Q / E_\omega$.

Introduce these new quantities to (2.4.20) and perform the integration, the density of states in tail region can be expressed in term of two dimensionless functions, $a(v, Z)$ and $b(v, Z)$ as follow²⁰

$$\rho_1(v, Z) = \frac{Q^3}{E_Q \xi^{5/4}} \frac{a(v, Z)}{(b(v, Z))^{3/4}} \exp(-b(v, Z) / 4\xi') D_{3/2}(\sqrt{b(v, Z) / \xi'}) \quad 2.4.21$$

where $a(v, Z) = \frac{(3/2Z^{-2} + v)^{3/2}}{8\pi\sqrt{2} Z^6 \exp(Z^2/2) D_{-3}^2(Z)}$, 2.4.22

$$b(v, Z) = \frac{\sqrt{\pi}(3/2Z^{-2} + v)^2}{2\sqrt{2} \exp(Z^2/4) D_{-3}(Z)}, \quad 2.4.23$$

and $\xi' = \xi / E_Q^2$. 2.4.24

Note that (2.4.21) is evaluated from (2.4.20) by using the formula¹¹

$$\int_{-\infty}^{\infty} dt (it)^P \exp(-\beta^2 t^2 - iqt) = 2^{-P/2} \sqrt{2} \beta^{-P-1} \exp(-q^2 / 8\beta^2) D_P(q / \sqrt{2}\beta) \quad 2.4.25$$

In the limit of large $b(v, Z) / \xi'$ the asymptotic expression for $\rho_1(v, Z)$

$$\text{is } \rho_1(v, Z) = \frac{Q^3}{E_Q \xi^2} a(v, Z) \exp(-b(v, Z)/2\xi'). \quad 2.4.26$$

This comes from the asymptotic expression for the parabolic cylinder function¹¹

$$D_p(Z) = \exp(-Z^2/4) Z^p (1 - \frac{p(p-1)}{2Z^2} + \dots). \quad 2.4.27$$

The parameter ω which is contained in Z has to be determined.

Following Halperin and Lax⁸ the parameter ω or Z must be chosen so that $\rho_1(v, Z)$ is maximized. For deep tail states $b(v, Z)/2\xi' \gg 1$ the exponential term in density of states dominates. To maximize $\rho_1(v, Z)$, we need only to maximize the exponential term by minimizing the function $b(v, Z)$ as Halperin and Lax⁸ did. There is another procedure of choosing an appropriate Z . This procedure is given by Lloyd and Best²¹ bases on mathematical theorem of variational principle. The three processes used to evaluate appropriate Z 's and the numerical values of density of states will be discussed in the next chapter

Another interesting point of this path integral method is that Kane's density of states can be obtained by considering only the high energies which corresponding to the limit $t \rightarrow 0$. From (2.4.18) and (2.4.19), if we take $t \rightarrow 0$ the density of states at high energies becomes⁹

$$\rho_1(E) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \left(\frac{m^*}{2\pi i \hbar t} \right)^{3/2} \exp\left(-\frac{\hbar^2 t^2}{4\pi^2} + \frac{i}{\hbar}(E - E_0)t\right),$$

where
$$n = \left(\frac{4\bar{N}}{Q}\right)^{1/2} \left(\frac{Ze^2}{\epsilon}\right).$$

This equation is equivalent to (2.2.12) which is derived from Kane's idea. Notice that the parameter Z or ω does not appear in the above equation.

Now let us pay attention to the quantity n defined as

$$n(v, Z) = \frac{\partial \ln b(v, Z)}{\partial \ln v} . \quad 2.4.29$$

In the path integral method this quantity is easily calculated. By using chain rule of differentiation (2.4.29) becomes

$$n(v, Z) = \frac{\partial \ln b(v, Z)}{\partial v} / \frac{\partial \ln v}{\partial v} .$$

Since the function $b(v, Z)$ is given by equation (2.4.23), we have

$$\begin{aligned} \frac{\partial \ln b(v, Z)}{\partial v} &= \frac{\partial}{\partial v} \left\{ 2 \ln \left(\frac{3}{2} Z^{-2} + v \right) \right. \\ &\quad \left. + \ln \left(\sqrt{\pi} / (2 \exp(Z^2/4) D_{-3}(Z)) \right) \right\} \\ &= 2 / \left(\frac{3}{2} Z^{-2} + v \right) . \end{aligned}$$

Then n will be obtain as

$$n(v, Z) = 2v / \left(\frac{3}{2} Z^{-2} + v \right) \quad 2.4.30$$

We can see that the values of $n(v, Z)$ can be evaluated easily if appropriate Z 's are known. The values and graphs of $n(v, Z)$ will be given in the next chapter.