

CHAPTER II

SEMICLASSICAL APPROACH

2.1 Introduction

As mentioned in chapter I, we consider the random effect as perturbation on the system which can be treated by perturbative technique. We found however that this method cannot explain the band tailing effect. Since this effect arises from the spatial fluctuations in the impurity density which correspond to negative fluctuations in the electronic potential, it does not appear that random effect can be treated as perturbation. The density of states can also be determined from the probability distribution of fluctuation. For non-perturbative technique, a semi-classical or Thomas Fermi method have been used by Kane.¹⁹

2.2 The Model Hamiltonian

¹⁹

Kane assumed the following model Hamiltonian

$$H = H_0 + H_1 \quad 2.2.1$$

$$H_1 = \sum_i V(\vec{r} - \vec{R}_i) - V_0 \quad 2.2.2$$

$$V(r) = -\frac{e^2}{\epsilon r} \exp(-Qr) \quad 2.2.3$$

$$H_0 = \frac{P^2}{2m} + C \quad 2.2.4$$

Here m is an effective mass of pure semiconductor, ϵ is

dielectric constant and $V(\vec{r})$ is assumed to be the screened Coulomb potential. V_0 is a constant chosen so that the average perturbing potential is zero.

2.3 Thomas - Fermi Assumption^{1,3}

Thomas suggested that when charges are introduced into the background while the net charge is zero, the energy of system would change by the amount given by Poisson's equation

$$\nabla^2 V = -4\pi \rho = -4\pi e(n_0(r) - n(r)) \quad 2.3.1$$

where $n(r)$ is the number density of electrons and $n_0(r)$ is the number density of background. We have

$$n_0(r) = c \sqrt{E} \quad 2.3.2$$

$$n(r) = c \sqrt{E - eV} \quad 2.3.3$$

Substituting (2.3.2) and (2.3.3) into (2.3.1), one obtains

$$\nabla^2 V = -4\pi e c \sqrt{E} \left(\left\{ 1 - \frac{eV}{E} \right\}^{1/2} - 1 \right) \quad 2.3.4$$

From (2.3.4), $\left\{ 1 - \frac{eV}{E} \right\}^{1/2}$ can be expanded in Taylor series.

Keeping only the first two terms, one obtains

$$V(r) = \frac{-e}{r} e^{-rQ} \quad 2.3.5$$

where Q is the reciprocal screening length.

Kane used the assumptions in the semiclassical method. The first one is that an electron-impurity potential is slowly varying, i.e., or the potential is smoothed. The other is the local density of states at point \vec{r} is given by the free electron density of states where the potential is given at the local value throughout the system. These assumptions are valid for states that are high in the bands but may not be true for localized states (ground states).

2.4 Semiclassical Approximation^{19,21}

The free electron density of states is given by (1.1.23)

$$\text{as } \rho(E) = \frac{\sqrt{2} m^{3/2}}{\pi^2 \hbar^3} \sqrt{E} H(E) \quad 2.4.1$$

Kane made the approximation that the number of states per unit energy range in $\Delta\Omega$ which is a small volume is given by

$$\rho(E-V) = (\sqrt{2} m^{3/2} / \pi^2 \hbar^3) (E-V)^{1/2} H(E-V) \quad 2.4.2$$

where $H(E-V)$ is defined by

$$\begin{aligned} H(E-V) &= 1 & E > V \\ &= 0 & E < V \end{aligned}$$

The density of states of the random system are obtained by taking an average over all configurations. Thus the density of states is obtained by using the probability densities $P(V)$ as

$$\rho(E) = \langle \rho(E-V) \rangle_V \quad 2.4.3$$

By using (2.4.2), $\rho(E)$ can be rewritten as

$$\begin{aligned} \rho(E) &= \frac{\sqrt{2} m^{3/2}}{\pi^2 h^3} \int_{-\infty}^{\infty} dV P(V) \sqrt{E - V} H(E - V) \\ &= \frac{\sqrt{2} m^{3/2}}{\pi^2 h^3} \int_{-\infty}^E dV P(V) \sqrt{E - V} \end{aligned} \quad 2.4.4$$

2.5 The Potential Distribution Function ^{19,20}

The impurity potentials are defined by

$$V = V(\vec{r}) = \sum_i^N V(\vec{r} - \vec{R}_i) \quad 2.5.1$$

where $V(\vec{r} - \vec{R}_i)$ is the potential due to a donor or an acceptor at position \vec{R}_i which is assumed to be random. Thus the probability distribution of \vec{R}_i , which is the probability that \vec{R}_i is in $d\vec{R}_1$, \vec{R}_2 is in $d\vec{R}_1, \vec{R}_2$ is in $d\vec{R}_2 \dots$ etc is $d\vec{R}_1/\Omega, d\vec{R}_2/\Omega \dots, d\vec{R}_N/\Omega$ where Ω is volume of system, is given by

$$P(\vec{R}_1 \dots \vec{R}_N) = \frac{d\vec{R}_1 \dots d\vec{R}_N}{\Omega^N} \quad 2.5.2$$

where N is the number of impurities. We note that (2.5.2) is suitable for describing the statistical properties of the impurities in a heavily doped semiconductor where N is large. Assuming that even with the highest concentrations the impurities are far enough apart for the probability of overlap to be negligible, the probability distribution can be treated

as statistically independent. The Fourier transform of Gaussian distribution of $P(V)$ for potential fluctuation of magnitude V is defined by

$$P(\alpha) = \int_{-\infty}^{\infty} \exp(i\alpha V) P(V) dV \quad 2.5.3$$

$$P(V) = \int_{-\infty}^{\infty} \exp(-i\alpha V) P(\alpha) \frac{d\alpha}{2\pi} \quad 2.5.4$$

Then from (2.5.3)

$$P(\alpha) = \int \dots \int \exp \left\{ i\alpha \sum_i V(\vec{r} - \vec{R}_i) \right\} \cdot \frac{d\vec{R}_1 \dots d\vec{R}_N}{\Omega^N}$$

Since the probability distribution is statistically independent, (2.5.5) can be written as

$$P(\alpha) = \left\{ \int \exp(i\alpha V(\vec{r} - \vec{R})) \frac{d\vec{R}}{\Omega} \right\}^{n\Omega} \quad 2.5.6$$

where $\frac{N}{\Omega} = n$ is defined as donor or acceptor concentrations.

$$\text{Since } \int_{\Omega} e^{i\alpha V(\vec{r}-\vec{R})} \frac{d\vec{R}}{\Omega} = 1 + \int_{\Omega} (e^{i\alpha V(\vec{r}-\vec{R})} - 1) \frac{d\vec{R}}{\Omega} \quad 2.5.7$$

$$\text{one notes that } \lim_{N \rightarrow \infty} \left(1 + \frac{X}{\Omega}\right)^N = e^X \quad 2.5.8$$

By using (2.5.7) and (2.5.8), (2.5.6) becomes

$$P(\alpha) = \left\{ n \int (\exp(i\alpha V(\vec{r} - \vec{R})) - 1) \frac{d\vec{R}}{\Omega} + 1 \right\}^{n\Omega} \quad 2.5.9$$

$$= \exp \left\{ n \int (\exp i\alpha V(\vec{r} - \vec{R}) - 1) d\vec{R} \right\} \quad 2.5.10$$

Since the expansion of e^x is equal to $1 + x + \frac{x^2}{2!} + \dots$

Equation (2.5.10) becomes

$$P(\alpha) = \exp \left\{ n \int (i\alpha V(\vec{r} - \vec{R}) - \frac{1}{2} \alpha^2 V^2(\vec{r} - \vec{R}) + \dots) d\vec{R} \right\} \quad 2.5.11$$

We now consider in the limit when $V \rightarrow 0$, $n \rightarrow \infty$ so nV^2 is finite and $nV^3 \ll nV^2$:

Substituting $P(\alpha)$ into (2.5.4) one obtains

$$P(V) = \int_{-\infty}^{\infty} e^{-i\alpha V} \frac{d\alpha}{2\pi} e^{n \int (i\alpha V(\vec{r} - \vec{R}) - \frac{1}{2} \alpha^2 V^2(\vec{r} - \vec{R})) d\vec{R}} \quad 2.5.12$$

In case of heavily doped semiconductor, the appropriate potential are assumed to be the screened Coulomb potential

$$V(\vec{r} - \vec{R}) = \frac{-e^2}{\epsilon |\vec{r} - \vec{R}|} e^{-Q |\vec{r} - \vec{R}|} \quad 2.5.13$$

where ϵ is the static dielectric constant and Q^{-1} is the screening length which is independent of impurity position. Performing the integration, we get

$$\int d\vec{R} V(\vec{r} - \vec{R}) = - \frac{4\pi e^2}{\epsilon Q^2}$$

$$\text{and} \quad \int d\vec{R} V^2(\vec{r} - \vec{R}) = \frac{2\pi e^4}{\epsilon^2 Q} \quad 2.5.14$$

$$\text{Letting} \quad V_0 = - \frac{4\pi e^2}{\epsilon Q^2} \quad 2.5.15$$

we get $\xi = \left(\frac{4\pi n}{Q}\right)^{1/2} \frac{e}{\epsilon}$ 2.5.16

Replacing (2.5.15) and (2.5.16) into (2.5.12), we obtain

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\alpha V} e^{V_0 - 1/4 \alpha^2 \xi^2} d\alpha \quad 2.5.17$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\alpha(V - V_0) - 1/4 \alpha^2 \xi^2} d\alpha \quad 2.5.18$$

We have standard formula. ²²

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

Thus the distribution $P(V)$ for the potential of (2.5.13) in the high density limit given by Kane is

$$P(V) = \frac{1}{\sqrt{\pi}} \frac{e^{-(V-V_0)^2/\xi^2}}{\xi} \quad 2.5.19$$

2.6 Density of States

The density of states which is obtained by substituting $P(V)$ into (2.4.4) may then be rewritten as

$$\begin{aligned} \rho(E) &= \int_{-\infty}^E \frac{\sqrt{2m}}{\pi \hbar^3} \frac{1}{\sqrt{\pi}} \frac{e^{-(V-V_0)^2/\xi^2}}{\xi} \sqrt{E-V} dV \\ &= \frac{2}{\pi \hbar^3 \xi \pi} \frac{1}{2} \int_{-\infty}^E e^{-(V-V_0)^2/\xi^2} \sqrt{E-V} dV \quad 2.6.1 \end{aligned}$$

For $E \rightarrow \infty$ (2.6.1) can be written as

$$\rho(E) = \frac{2^{1/2} m^{3/2}}{\pi^2 \hbar^3 \sqrt{\pi} \xi} \int_{-\infty}^{\infty} e^{-(V-V_0)^2/\xi^2} \sqrt{E} dV \quad 2.6.2$$

Using the standard formula

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$$

Then (2.6.2) may be written as

$$\rho(E) = \frac{2^{1/2} m^{3/2}}{\pi^2 \hbar^3} \sqrt{E} \quad 2.6.3$$

and (2.6.3) is the density of states of an unperturbed band

From (2.6.1) if one changes the variable $E - V = y$, then

$$dy = -dV$$

and the limit of integration ($E, -\infty$) must be changed to ($0, \infty$).

One then gets

$$\begin{aligned} \rho(E) &= \frac{2^{1/2} m^{3/2}}{\xi \pi^2 \hbar^3 \pi^{1/2}} \int_{+\infty}^0 dy \sqrt{y} e^{-(E-y-V_0)^2/\xi^2} \\ &= \frac{2^{1/2} m^{3/2}}{\xi \pi^2 \hbar^3 \pi^{1/2}} e^{-(E-V_0)^2/\xi^2} \int_0^{\infty} dy \sqrt{y} e^{2(E-V_0)/\xi^2 - y^2/\xi^2} \\ \rho(E) &= \frac{2^{1/2} m^{3/2}}{\xi \pi^2 \hbar^3 \pi^{1/2}} e^{-(E-V_0)^2/\xi^2} \int_0^{\infty} dy \sqrt{y} e^{2(E-V_0)/\xi^2 - y^2/\xi^2} \quad 2.6.4 \end{aligned}$$

By using the formula ²²

$$\int_0^{\infty} x^{\nu-1} e^{-\beta x^2 - \xi x} dx = (2\beta)^{-\nu/2} \Gamma(\nu) \exp\left(\frac{\xi^2}{8\beta}\right) D_{-\nu}\left(\frac{\xi}{2\beta}\right)$$

(2.6.4) may be written in the form of parabolic cylinder function as

$$\rho(E) = \frac{1}{\pi} \sqrt{\frac{m}{h^3}} \cdot 2^{-7/4} \xi^{3/2} D_{-3/2}\left(\frac{-\sqrt{2}(E-V_0)}{\xi}\right) e^{-(E-V_0)^2/2\xi^2} \quad 2.6.5$$

Writing

$$x = \frac{(E-V_0)}{\xi}$$

$$\rho(E) = \frac{1}{\pi} \sqrt{\frac{m}{h^3}} \cdot 2^{-7/4} \xi^{1/2} \exp(-x^2/2) D_{-3/2}(-\sqrt{2} x) \quad 2.6.6$$

Kane considered function

$$y(x) = 2^{-7/4} \exp(-x^2/2) D_{-3/2}(-\sqrt{2} x) \quad 2.6.7$$

This function is plotted in Fig 2.1 and Fig 2.2. For $E \rightarrow \infty$, one ²³ uses the asymptotic properties of parabolic cylinder function, i.e.,

$$D_{\nu}(X) \sim \exp(-X^2/4) X^{\nu} \quad X \gg |\nu|$$

and obtains $y(x) \sim \sqrt{x}$. For $E \rightarrow -\infty$, the asymptotic properties ²³ of parabolic cylinder, i.e.,

$$D_v(-X) \sim \sqrt{2\pi} e^{-x^2/4} X^{-v-1} \quad X \gg |v|$$

we obtain $y(x) \approx e^{-x^2/2}$

It is noticed that because of the Gaussian statistics of the potential, the density of states in the low energy forms a band tail of Gaussian form. Thus the semiclassical method gives energy states which are too low. As a result it overestimates tail length. Kane concluded that this is due to neglect the effect of the kinetic energy of localization in deriving (2.5.19). However the method has proved to be useful on description of the band shape in heavily doped semiconductor.

Kane's method always gives the deep tail states which is in the form of $\exp(-E^2)$. But experiments show that deep tail states in the form $\rho \sim \exp(-E^n)$ with n vary from $\frac{1}{2}$ to 2 Halperin and Lax²⁴ and Sayakanit³¹ proposed the theory that can correct this failure.

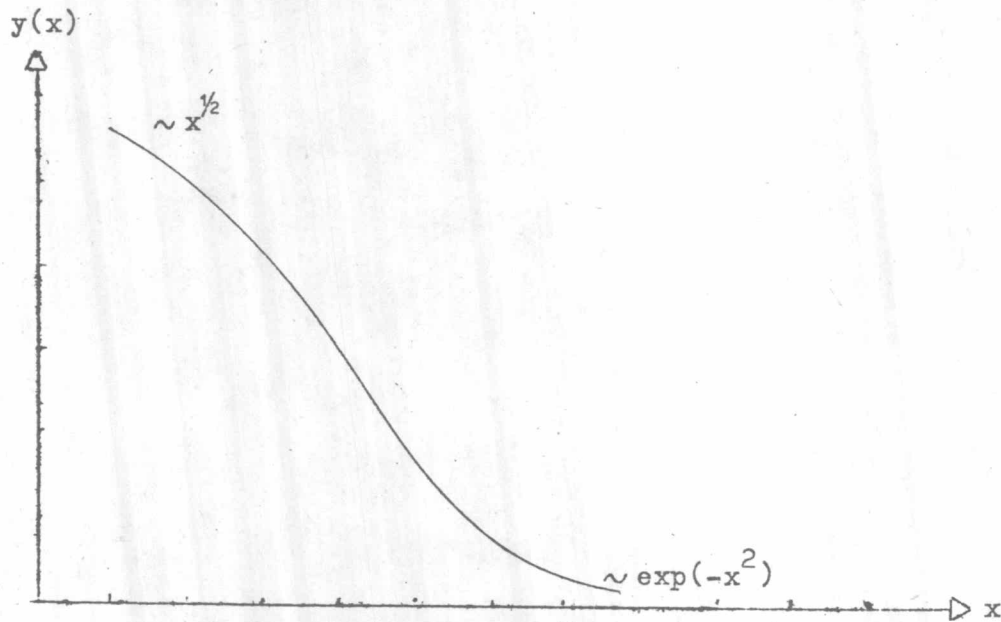


Fig 2.1 Thomas - Fermi density of states versus energy
in dimensionless variables

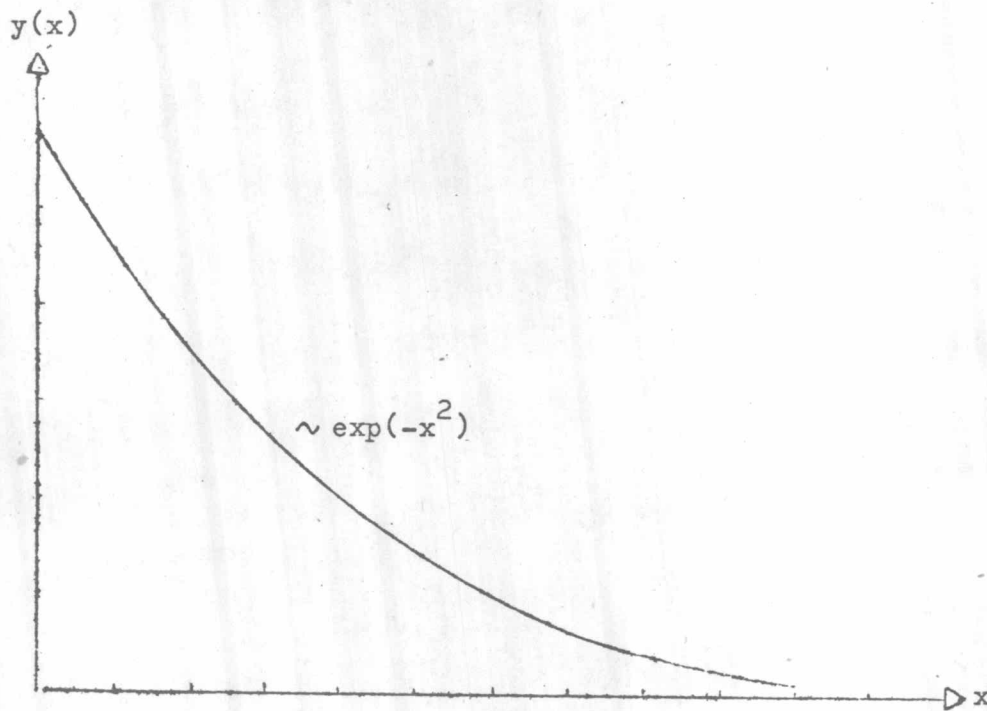


Fig 2.2 Density of states versus energy in dimensionless
variables(Tail states)