CHAPTER III

QUANTUM THEORETICAL APPROACH

3.1 Introduction

As mentioned in chapterII, the Kane's theory leads to an overestimation of tail states. This failure arises from the use of semiclassical model which neglects the kinetic energy of localization (zero point energy). Quantum mechanical theory yields several different approaches, i.e., the method of Shrödinger (wave mechanics), the method of Feynman (Path Integral theory)[27] etc. Halperin and Lax[24] used " Wave Mechanics" successfully in describing the deep tail states in heavily doped semiconductor. Sa-yakanit[31] used Feynman's method on this problem and obtained the same results. In this chapter we will mention only the work of Halperin and Lax. They have proposed a new theory that is of a non perturbation nature and have obtained a good estimation of states in the low energy tail where the density of states is small. The method is based on quantum mechanical theory. They have obtained their results for a potential distribution obeying Gaussian statistics.

3.2 The Hamiltonian Model[24,26]

Halperin and Lax consider a model in which the Hamiltonian is described by

$$H = H_o + \tilde{V}(\vec{r})$$

where

$$H_o = \frac{-\bar{h}^2}{2m} \nabla^2$$

$V(\vec{r})$ is the random fluctuating potential with mean $\langle V \rangle_v = E_o$. $\tilde{V}(\vec{r})$ is randomly spaced wells of random depths and shape This is shown in Fig.3.1.

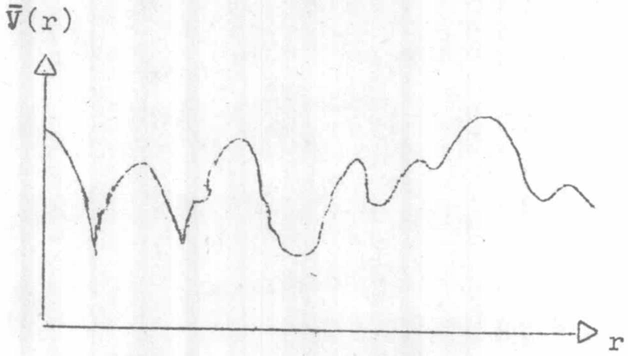

Fig 3.1 Random nature of potential V(r) against r in an amorphous material.

Let us write $V(\vec{r}) = \tilde{V}(\vec{r}) - E_o$. Then the Hamiltonian becomes

$$H = T + \tilde{V}(\vec{r}) \qquad 3.1.1$$

$$= \frac{-\bar{h}^2}{2m} \nabla^2 + E_o + V(\vec{r}) \qquad 3.2.2$$

The kinetic energy term represents the energy of an electron in pure crystal. $V(\vec{r})$ is the random potential represents the difference between the impurity pseudopotentials and pure host psuedopotentials. Halperin and Lax assume that $V(\bar{r})$ is the sum of individual impurity potentials

3.3 The Low Energy Tail^{24,25}

Let E_1 be the energy of the ground state of an impurity

If the system is dilute so that the overlap of the wave functions is small, then there will be states close to E_1. For the energy belows E_1, we will consider the cluster of two impuritics and so on as shown in Fig 3.2.

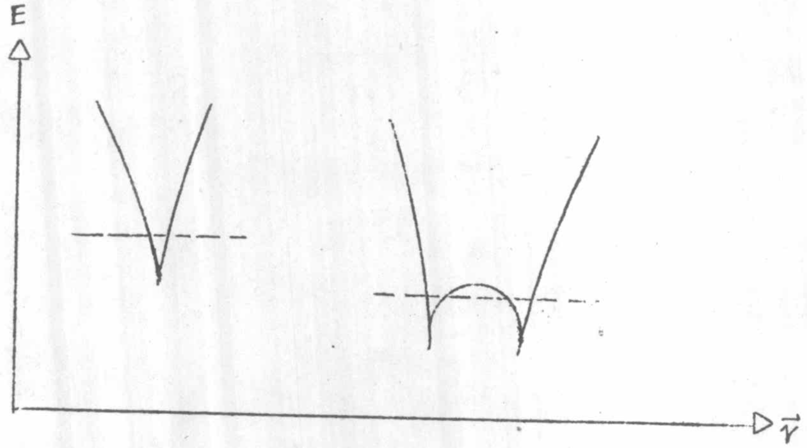

Fig 3.3 Schematic drawing of potential V(x) (solid curve) and low lying energy levels (broken lines)

Assumming that the low energy tail arises from the fluctuations of many impurities within the range of wave function, the tail states must depend on the shape of impurity potential wells.

3.4 The Kinetic Energy of Localization [24,25,33]

As is well known in the semiclassical approximation, the ground state energy is located at the bottom of the wells. This means that theory of Kane places the states which are too low. Therefore it predicts the too lengthening tail. According to the quantum model, if the size of well is large the zero point energy will lie near to the bottom of the well. On the other hand, if the well is small it will lie much above the bottom of the well.

Thus the zero point energy depends on the shape of the well as shown in Fig 3.3.

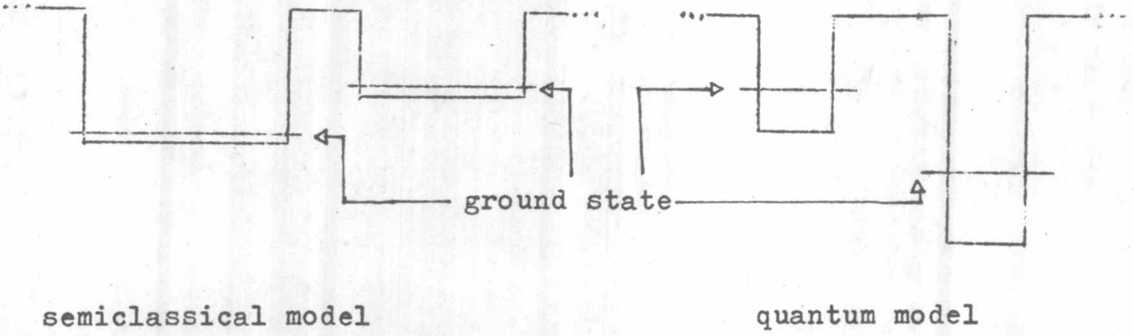

Fig 3.3 The difference of the level of the kinetic energy of localization between two models

3.5 The Eigen State[24,25]

According to the quantum theory there is a correspondence between the wave function and the eigen energy E for each state. Halperin and Lax assume a one to one correspondence between the wave function and energy in the tail. They also assume that the width of wave function is large compared with the range of an impurity potential. As mentioned in Sec(3.4), the narrower of the wave function the larger of kinitic energy of localization will be. So the problem is to find an appropriate wave function which is not too narrow and not too spread and assume that they have approximately the same shape in the low energy tail. To determine the shape of wave functions one looks that the statistics of the impurity potentials introduce the most probable shape at energy E. Suppose we know the wave function $\psi_i(\vec{r})$, we can determine the eigen value $E_i = E$.

But in fact we do not know the shape of $\psi_i(\vec{r})$. However in quantum theory it can be assumed that $\psi_i(\vec{r})$ has the form of the real, normalized function

$$\psi_i(\vec{r}) \simeq f(\vec{r} - \vec{y}_i) \tag{3.5.1}$$

with

$$\int f^2(r-\vec{y}_i)d\vec{r} = 1 \tag{3.5.2}$$

where the fixed function $f(\vec{r}-\vec{y}_i)$ is the corresponding wave function of the well that locates at $\vec{y}_i$ which is different for each eigen states. One may assume that each eigen energy E_i will correspond to each point $\vec{y}_i$. If one treat $f(\vec{r}-\vec{y}_i)$ as a trial wave function of the Hamiltonian of the system , the Schrödinger equation will be

$$H\, f\, (\vec{r}-\vec{y}_i) = E\, (\vec{y}_i) f\, (\vec{r}-\vec{y}_i) \tag{3.5.3}$$

where $$E(\vec{y}_i) = \int f(\vec{r}-\vec{y}_i)\, H\, f(\vec{r}-\vec{y}_i)\, d\vec{r} \tag{3.5.4}$$

Substituting the value of H from (3.1.1) we get

$$E(\bar{y}_i) = \int f(\vec{r}-\vec{y}_i)(-\frac{\bar{h}^2}{2m}\nabla^2)\, f(\vec{r}-\vec{y}_i)d\vec{r} + V_o$$

$$+ \int f(\vec{r}-\vec{y}_i)\, V(\vec{r})\, f(\vec{r}-\vec{y}_i)d\vec{r} \tag{3.5.5}$$

$$= T_s + V_o + V_s(\vec{y}_i) \tag{3.5.6}$$

where $V_s(y)$ represents the potential energy $V(\vec{r})$ smoothed by the square of the wave function.

Here T_s and $\hat{V}_s$ are defined from

$$T_s = \langle f | T | f \rangle = \int f(\vec{r}-\vec{y}) T \, f(\vec{r}-\vec{y}_i') d\vec{r} \qquad 3.5.7$$

and the smoothed potential is defined

$$V_s(\vec{y}_i) = \langle f | V(\vec{r}) | f \rangle = \int f^2(\vec{r}-\vec{y}) V(\vec{r}) \, d\vec{r} \qquad 3.5.8$$

One notes that the kinetic energy term is translational invariant. $V_s(\vec{y}_i)$ is the average of the potential $V(\vec{r})$ in a region about $\vec{r} = \vec{y}_i$ .As $\vec{y}$ is varied throughout the system, $V_s(\vec{y})$ will fluctuate about an average value of $\langle V(\vec{r}) \rangle$, and at some places $V_s(\vec{y})$ will show large negative fluctuations. Since these places correspond to regions of very low $V(\vec{r})$ one expects to find a low-energy eigen state $\psi_i(\vec{r})$. One knows that a variational estimate of the ground state energy of a system always overestimates this energy. Hence, one expects that $E(\vec{y}_i)$ which is in a region of negative fluctuations will often be larger than the true energy E_i of the local low energy eigenstate. The best estimate of the energy E_i is thus obtained by choosing $\vec{y}$ so that $E(\vec{y})$ is as small as possible that means $E(\vec{y}_i)$ is a local minimum and equivalents to the point where

$$\nabla E(\vec{y}) = 0 \qquad 3.5.9$$

Since E(y) is only depend on potential term, one can consider

$$\nabla V_s(y) = 0 \qquad 3.5.10$$

3.6 The minimum counting method

In the low-energy tail, where the density of states is very small, energy eigenstates are few and for between and the possibility of overlap between $f(\vec{r}-y_i)$ and two different eigenstates is negligible. Therefore, there is a close one to one correspondence between local minima in E(y) and the energy of eigenstates in the vicinity of E. Then the number of eigenstates with Energy E is approximately equal to the number of local minima in E(y) with value E. Thus one has the following approximation to the density of states

$$\rho_f(E) = \frac{1}{\Omega dE} \langle \text{(number of local minima in } E(y) \text{ in the interval } (E, E+dE) \rangle \qquad 3.6.1$$

where one notes that at the minimum $E < E(y) < E + dE$ and Ω = the volume of the crystal.

Let us now consider the problem of finding the best trial function f . One knows that regardless of the choice of f, the variational estimates of the energies of the eigenstates will be high. In the low-energy tail where the density of states decreased rapidly, this overestimate of all the eigenstates gives an underestimation of the density of states. Thus the best choice of f, for any given energy E is that which maximizes $\rho(E)$, so that one has

$$\rho_1(E) = \max_f(\rho_f(E)) \qquad 3.6.2$$

3.7 The Density of States.[24,25,37]

To evaluate $\rho_1(E)$, we begin with the definition of density of states of the random system as given in chapter II, i.e.,

$$\rho(E) = \frac{1}{\Omega} < \Sigma\,\delta(E-E_i(V)) >_V \qquad 3.7.1$$

We note that the above formula has already been average since E_i depends on V which is random. Next we substitute (3.5.6) into (3.7.1) and obtain

$$\rho_f(E) = \frac{1}{\Omega} < \Sigma\,\delta(E - \left[T_s + V_s(\vec{y}_i)\right]) >_V \qquad 3.7.2$$

By using the property that $\int f(\vec{y})\,\delta(\vec{y}-\vec{y}_i)\,dy = f(\vec{y}_i)$ the above equation may be written as

$$\rho_f(E) = \frac{1}{\Omega} \int dy < \sum_i \delta(\vec{y} - \vec{y}_i)\,\delta(E - [T_s + V_s(\vec{y})]) >_V \qquad 3.7.3$$

where $\vec{y}$ is any point in crystal and $\{\vec{y}_i\}$ is the set of points satisfying $\nabla V_s(\vec{y}_i) = 0$.

We note that the symbol $< \; >_V$ which appear in (3.7.2) is the average over $V_s(\vec{y})$. Since the average function is independent of $\vec{y}$, then the number of minima can be counted by

$$\rho_f(E) = < \sum_i \delta(\vec{y}-\vec{y}_i)\, \delta(E-T_s+V_s(\vec{y}_i)) >_{V_s(\vec{y})} \qquad 3.7.4$$

For convenience one makes the transformation from the variable y to $\nabla V_s(\vec{y})$ by writing

$$\sum_i(\delta(\vec{y}-\vec{y}_i)) = \delta(\nabla V_s(\vec{y})) \det\left|\nabla\nabla V_s(\vec{y})\right| \qquad 3.7.5$$

where $\det|\nabla\nabla V_s(\vec{y})|$ arises from the Jacobian transformation

Substituting (3.7.5) into (3.7.4) and one gets

$$\rho_f(E) = <\delta(E-T_s-V_s(\vec{y}))\delta(\nabla V_s(\vec{y}))|\det \nabla\nabla V_s(\vec{y})| > \qquad 3.7.6)$$

$$\rho_f(E) = \int P(V_s(\vec{y}))\, \delta(\lambda-V_s(\vec{y}))P(V_s(\vec{y})\,|\,\nabla V_s(\vec{y}))|\delta(\nabla V_s(\vec{y})-\Delta)\,|\nabla\nabla V_s(\vec{y})|\; dV_s(\vec{y})d\nabla V_s(\vec{y}) \qquad (3.7.7)$$

where $\lambda = (E-T_s)$ and $\Lambda = 0$. (3.7.7) can be written as the product of three factors of joint probability

$$\rho_f(E) = P(\lambda)\, P_3(\Lambda|\lambda)\chi(\lambda,\Lambda) \qquad (3.7.8)$$

where $P(\lambda)$ is the probability density for $V_s(\vec{y})$ having the value λ at point y. $P_3(\Lambda|\lambda)$ is the conditional probability density for $\nabla V_s(\vec{y})$

having the value Λ when one conditions $V_s(\vec{y}) = \lambda$. $\chi(\lambda,\Lambda)$ is the conditional expectation value of det $\nabla\nabla V_s(\vec{y})$ when one requires $V_s(\vec{y}) = \lambda$ and $\nabla V_s(\vec{y}) = \Lambda$.

To calculate $\rho_f(E)$ one needs to know the statistical properties of the random potential V. If the system is statistically homogeneous then

$$\langle V(\vec{r})\rangle = \bar{V} \tag{3.7.9}$$

where $\bar{V}$ is a constant independent of $\vec{r}$ and the two points auto correlation function of the original function of $V(\vec{r})$ is given by

$$\langle V(\vec{r})V(\vec{r}')\rangle = \eta^2\bar{N}\int v(\vec{r}-\vec{R})v(\vec{r}'-\vec{R})\,d\vec{R}$$

From the relation between $V_s(\vec{y})$ and $V(\vec{r})$ (3.5.8), the autocorreclation function $\langle V_s(\vec{y})\,V_s(\vec{y}')\rangle$ can be written as

$$\langle V_s(\vec{y})V_s(\vec{y}')\rangle = \int f^2(\vec{r}-\vec{y})f^2(\vec{r}'-\vec{y}')\langle V(\vec{r})V(\vec{r}')\rangle d\vec{r}\,d\vec{r}' \tag{3.7.10}$$

Halperin and Lax define

$$\xi = \eta^2\bar{N}$$

Then the above expression may be written as

$$\langle V(\vec{r})V(\vec{r}')\rangle = \xi W(\vec{r}-\vec{r}') \tag{3.7.11}$$

where $$W(\vec{r}-\vec{r}') = \int V(\vec{r}-\vec{R})V(\vec{r}'-\vec{R})\,d\vec{R} \tag{3.7.12}$$

and similarly

$$<V_s(\vec{y})V_s(\vec{y}')> \quad = \quad \xi G(\vec{y}-\vec{y}') \qquad (3.7.13)$$

where $$G(\vec{y}-\vec{y}') \quad = \quad \int f^2(\vec{r}-\vec{y})f^2(\vec{r}-\vec{y}')w(\vec{r}-\vec{r}')d\vec{r}\,d\vec{r}' \qquad (3.7.14)$$

In the case of heavily doped semiconductors the impurity concentrations $\bar{N}$ is very high and so the distribution of impurity obeys Gaussian statistics. If Gaussian statistics are assumed, then $P(\lambda)$ can be written as

$$P(\lambda) \;=\; P(V_s(\vec{y}) = E-T_s) \;=\; (2\pi\,\xi\sigma_o^2)^{-1/2}\exp(-\lambda^2/2\,\xi\sigma_o^2) \qquad (3.7.15)$$

where the variance $\xi\sigma_o^2 \;=\; <V_s^2(\vec{y})> \;=\; \xi G(o)$ (3.7.16)

To determine $P(\Lambda|\lambda) \;=\; P(\nabla V_s(\vec{y}) = 0 \mid V_s(\vec{y}) = E-T_s)$ one considers the covariance $V_s(\bar{y})$ with $\nabla V_s(\bar{y})$ by differentiate(3.7.13) with respect to $\vec{y}'$ and set $\vec{y} = \vec{y}'$, one gets

$$<V_s(\vec{y})\nabla V_s(\vec{y}')> \;=\; \xi\nabla_{\vec{y}'}G(\vec{y}-\vec{y}')\Big|_{\vec{y}=\vec{y}'} = \;\xi\nabla_{\vec{y}}G(0) \qquad (3.7.17)$$

$$= \quad 0$$

The above property follows because $\nabla V_s(\vec{y})$ and $V_s(\vec{y})$ are statistically independent. Next we consider the covariance of $\nabla V_s(\vec{y})$ with itself by differentiate (3.7.13) twice and set $\vec{y} = \vec{y}'$, one gets

$$< (\nabla V_s(\vec{y}))\,(\nabla V_s(\vec{y})) > \;=\; -\xi\nabla\nabla G(o) \qquad (3.7.18)$$

If we let i,j represent the perpendicular axes1,2,and3the value of the variance $-\xi\nabla\nabla G(o)$ in each components may be written as

$$\sigma_i^2 = \sum_{ij} \frac{\partial^2}{\partial\vec{y}_i\,\partial\vec{y}_j} V_s(\vec{y}) \quad \text{or} \quad \sum_{ij} \frac{\partial^2 G(o)}{\partial\vec{y}_i\,\partial\vec{y}_j} \qquad (3.7.19)$$

The axes are chosen so that the matrix is diagonal with the form

$$\nabla\nabla G(O) = \begin{Bmatrix} \sigma_1^2 & 0 & 0 \\ 0 & \sigma_2^2 & 0 \\ 0 & 0 & \sigma_3^2 \end{Bmatrix} \qquad (3.7.20)$$

The product of three Gaussian conditional probability may be written in the form

$$P_3(\Lambda|\lambda) = \frac{e^{-\Lambda_1^2/2\xi\sigma_1^2}}{(2\pi\xi)^{1/2}\sigma_1} \cdot \frac{e^{-\Lambda_2^2/2\xi\sigma_2^2}}{(2\pi\xi)^{1/2}\sigma_2} \cdot \frac{e^{-\Lambda^2/2\xi\sigma_3^2}}{(2\pi\xi)^{1/2}\sigma_3}$$

$$= (2\pi\xi)^{-3/2} \exp\left(-\frac{\Lambda_1^2}{2\xi\sigma_1^2} - \frac{\Lambda_3^2}{2\xi\sigma_3^2} - \frac{\Lambda_2^2}{2\xi\sigma_2^2}\right)\sigma_1\sigma_2\sigma_3 \qquad (3.7.21)$$

Since $\Lambda = 0$, (3.7.21) becomes

$$P_3(0|\lambda) = (2\pi\xi)^{-3/2}(\sigma_1\sigma_2\sigma_3)^{-1} \qquad (3.7.22)$$

Next we consider $\chi(\lambda,\Lambda)$. The term $\nabla\nabla V_s(\vec{y})$ can be written in the form

$$\nabla\nabla V_s(\vec{y}) = V_s(\vec{y})M + X \tag{3.7.23}$$

where M is a constant matrix, X is variable matrix uncorrelated with $V_s(\bar{y})$. Multiplying (3.7.23) by $V_s(\vec{y})$, we obtain

$$V_s(\vec{y})\nabla\nabla V_s(\vec{y}) = V_s^2(\vec{y})M + XV_s(\vec{y}) \tag{3.7.24}$$

To determine $\chi(\lambda;\Lambda)$, (3.7.24) will be averaged

$$<V_s(\vec{y})\ \nabla\nabla V_s(\vec{y})> = <V_s^2(\vec{y})M> + <XV_s(\vec{y})>$$

Since $V_s(\vec{y})$ and X are statistically independent, i.e., one is deep in the tail, $<XV_s(\vec{y})> = 0$

Therefore
$$M = \frac{<V_s(\vec{y})\ \nabla\nabla V_s(\vec{y})>}{<V_s^2(\vec{y})>} \tag{3.7.25}$$

Considering $\nabla\nabla V_s(\vec{y})$ in each component one may write

$\sum_{ij} \frac{\partial^2 V_s}{\partial y_i \partial y_j}$ and diagonalize this matrix, one get determinant

$$\nabla\nabla V_s(\bar{y}) = \begin{vmatrix} \sigma_1^2 & 0 & 0 \\ 0 & \sigma_2^2 & 0 \\ 0 & 0 & \sigma_3^2 \end{vmatrix} \tag{3.7.26}$$

By using the condition $V_s(\vec{y}) = E-T_s$ and variance

$$< V_s(\vec{y}) > = \xi\sigma_0^2$$

One obtain

$$M = \frac{\frac{(E-T_s)^3}{6}}{\xi\sigma_o} \sigma_1^2 \sigma_2^2 \sigma_3^2 = \chi(\lambda,\Lambda) \qquad (3.7.27)$$

When (3.7.15), (3.7.22), and (3.7.27) are substituted into (3.7.8), we get

$$\rho_f(E) = \frac{\sigma_1\sigma_2\sigma_3(T_s-E)^3}{(2\pi)^2\xi^2\sigma_o^7} \exp\left[-(T_s-E)^2/2\xi\sigma_o^2\right] \qquad (3.7.28)$$

Let $B(E) = (T_s-E)^2/\sigma_o^2$ (3.7.29)

and $A(E) = \sigma_1\sigma_2\sigma_3(T_s-E)^3/2\pi^2\sigma_o^7$ (3.7.30)

then

$$\rho_f(E) = \frac{A(E)}{\xi^2} \exp(-B(E)/2\xi) \qquad (3.7.3)$$

Since $\rho(E) = \max \rho_f(E)$, Halperin and Lax maximize $\rho_f(E)$ by minimizing B(E).

Considering

$$\Gamma(E,f) = \frac{(E-T_s)^2}{\sigma_o^2} = \frac{\left(E - \int f(\vec{r})Tf(\vec{r})\,d\vec{r}\right)^2}{\int f^2(\vec{r})f^2(\vec{r}')W(\vec{r}-\vec{r}')\,d\vec{r}\,d\vec{r}'} \qquad (3.7.32)$$

with $\int f^2(\vec{r})\,d\vec{r} = 1$

then

$$\Gamma(E,f) = \frac{\left(\int E f^2(\vec{r})\,d\vec{r} - \int f(\vec{r})Tf(\vec{r})\,d\vec{r}\right)^2}{\int f^2(\vec{r})f^2(\vec{r}')W(\vec{r}-\vec{r}')\,d\vec{r}\,d\vec{r}'} \qquad (3.7.33)$$

Let $J^2 = \left\{ \int E\, f^2(\vec{r})d\vec{r} - \int f(\vec{r})Tf(\vec{r})d\vec{r} \right\}^2$; $N = \int f^2(\vec{r})w(\vec{r}-\vec{r}\,')d\vec{r}d\vec{r}\,'f^2(\vec{r}\,')$

Let us vary the function $f(\vec{r})$. This will induce changes $\delta\Gamma$, δJ , δN such that

$$\delta\Gamma = \frac{(J+\delta J)^2}{N+\delta N} - \frac{J^2}{N} = \frac{J^2 + 2J\delta J + (\delta J)^2}{N+\delta N} - \frac{J^2}{N}$$

$$= \frac{NJ^2 + 2JN\delta J + N(\delta J)^2 - J^2N - J^2\delta N}{N(N+\delta N)}$$

For some particular f(r) the value of Γ is stationary. Then

$$\delta\Gamma = 2JN\delta J + N(\delta J)^2 - J^2\delta N = 0$$

since $(\delta J)^2$ is small , we obtain

$$\delta J - \frac{J}{2N}\delta N = 0$$

One can replace $J/_N$ by $-\mu$, and the condition of extremum becomes $\delta J + \frac{\mu}{2}\delta N = 0$. Since

$\frac{\delta J}{\delta f} = \int E\, f(\vec{r})d\vec{r} - \int Tf(\vec{r})d\vec{r}$; $\frac{\delta N}{\delta f} = 2\int f(\vec{r})f^2(\vec{r}\,')d\vec{r}\, d\vec{r}\,'$, we obtain

$$\int d\vec{r}\,\left(Ef(\vec{r}) - Tf(\vec{r}) + \mu f(\vec{r}) \int f^2(\vec{r}\,')d\vec{r}\,'\right) = 0$$

$$Ef(\vec{r}) - Tf(\vec{r}) + \mu f(\vec{r}) \int f^2(\vec{r}\,')d\vec{r}\,' = 0 \qquad (3.7.34)$$

This equation looks similar to the Hatree type equation and can be solved by iteration technique. One assumes a potential and obtains the wave function. Then one uses this wave function to obtain a better potential and repeats the procedure to obtain the appropriate wave function.

3.8 Screened Coulomb Potential[24]

Halperin and Lax assume a linear screening model to describe the potential of each impurity which is in the form

$$\eta v(\vec{r}-\vec{R}) = \frac{-ze^2}{\varepsilon\,|\vec{r}-\vec{R}|} \exp(-Q\,|\vec{r}-\vec{R}|) \qquad (3.8.1)$$

and

$$V(\vec{r}) = \frac{e^2}{\varepsilon\,|\vec{r}-\vec{R}|} \exp(-Q\,|\vec{r}-\vec{R}|) \qquad (3.8.2)$$

Substituting (3.8.2) into (3.7.11) and working with Fourier transform , the random position $\vec{R}$ can be integrated out and, (3.7.11) becomes

$$\langle V(\vec{r})V(\vec{r}\,')\rangle = \xi \exp(-Q\,|\vec{r}-\vec{r}\,'|) = \xi W(\vec{r}-\vec{r}\,') \qquad (3.8.3)$$

where

$$\xi = \frac{2\pi}{Q}\,\frac{e^4}{\varepsilon_o^2}\,\bar{N}z^2 \qquad (3.8.4)$$

Since $f(\vec{r})$ is assumed to be in the form of spherical symmetric function

$$f(r) = (4\pi)^{-1/2}\,\frac{S(r)}{r} \qquad (3.8.5)$$

where $r = |\vec{r}|$ and $S(r) = 0$ when $r = 0$ and $r = \infty$, that is the localized wave function. Eqs.(3.2.1, 3.8.3 and 3.8.5) are substituted into (3.7.34), one obtains the Hatree-type equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} - \mu U(r)\right) S(r) = (E-E_o)S(r) \qquad (3.8.6)$$

where

$$U(r) = \int_0^\infty K(r,r')S^2(r')dr' \qquad (3.8.7)$$

with $r = |\vec{r}|$ and $K(r,r') = \langle W(\vec{r}-\vec{r}')\rangle$ which is the average of the function $\exp(-Q\,|\vec{r}-\vec{r}'|)$ with respect to the angular co-ordinates of the variable r. One finds

$$\langle W(\vec{r}-\vec{r}')\rangle = \frac{1}{2}\int_{-1}^{1} \exp\ -Q(r^2+r'^2+2rr'\mu)^{\frac{1}{2}}\, d\mu = K(rr')$$

For evaluating the above integral we let $\vec{R} = (r^2+r'^2+2rr'\mu)^{1/2}$

then $$K(rr') = \frac{1}{2rr'}\int_{r-r'}^{r+r'} d\vec{R}\, \exp(-Q\vec{R}).\vec{R}$$

By using the formula $$\int_0^\infty xe^{ax}\, dx = e^{ax}\left(\frac{x}{a} - \frac{1}{x^2}\right)$$

the above integral becomes

$$K(rr') = \frac{1}{Qrr'}\, e^{-Qr_>}\left((r_> + Q^{-1})\sinh Qr_< - r_<\cosh Qr_<\right)$$

where $r_<$ = the smaller of the length r and r'

$r_>$ = the larger of the length r and r'

The function S(r) is required to vanish at $r=0$ and $r = \infty$. Eqs.(3.8.6) and (3.8.7) can be solved iteratively for a range of values of the parameter $E-E_o$. For each value of $(E-E_o)$, a trial function was first used for S(r) in eq.(3.8.7), then the values of V(r) so obtained were substituted in (3.8.6). The value of μ is varied until the solution S(r) of (3.8.6) satisfies the boundary conditions and the function S(r) thus obtained is used as a new trial function in (3.8.7). Finally S(r) is known, A(E) and B(E) can be calculated. For convenient Halperin and Lax introduce the dimensionless quantity i.e. $E_Q = \frac{\hbar^2 Q^2}{2m}$ and $\nu = \frac{(E_o - E)}{E_Q}$

3.7.31 becomes

$$\rho(\nu) = (E_Q^3 \, Q^3/\xi^2) a(\nu) \exp(- E_Q^2/2\xi) b(\nu)) \qquad (3.8.8)$$

Let $Q = \frac{\hbar^2}{2m} = 1$, then (3.8.6) becomes

$$\left\{ -\frac{d^2}{dr^2} - \mu U(r) \right\} S(r) = -\nu S(r) \qquad (3.8.9)$$

where $a(\nu) = A(E)$ and $b(\nu) = B(E)$ (3.8.9.1)

For determining $a(\nu)$ and $b(\nu)$, one considers (3.7.16) Upon using eq.(3.7.14) one gets $\sigma_o^2 = G(o) = \int_o^\infty f^2(r) U(r) dr$ (3.8.10)

Further using eq.(3.7.19), we obtain

$$\sigma_1^2 = -\frac{\partial^2 G(0)}{\partial y_1^2} = -\int_o^\infty \frac{\partial^2}{\partial y_1^2} f^2(r) \, U(r) dr$$

$$= -\frac{1}{3} \int_0^\infty \nabla^2 \left[f(r)\right]^2 U(r)dr$$

$$= -\frac{1}{3} \int_0^\infty \nabla^2 \left[\frac{S^2(r)}{r}\right] rU(r)dr \qquad (3.8.11)$$

We note that (3.7.34) has

$$\int dr\, f(r)Tf(r) - \int \mu f^2(r) \int f(r')^2 w(r-r')\, dr'\, dr = \int f(r)E\, f(r)\, dr$$

$$\int f^2(r)U(r)\, dr = \frac{T-E}{\mu} \qquad (3.8.12)$$

$$\nabla^2 \left\{ \int f^2(r)U(r)dr \right\} = 0$$

$$\int \nabla^2 \left\{f(r)\right\}^2 U(r)dr = \int f^2(r)\, \nabla^2 U(r)\, dr \qquad (3.8.13)$$

By using (3.8.13), (3.8.11) may be written as

$$\sigma_1^2 = -\frac{1}{3} \int_0^\infty \frac{S^2(r)}{r} \frac{d^2}{dr^2} rU(r)\, dr \qquad (3.8.14)$$

Since f(r) is spherical symmetric, $\sigma_1^2 = \sigma_2^2 = \sigma_3^2$ (3.8.15)

Note that T - E = - potential energy

Eq(3.8.12) may be written as $T - E = \mu \int f,Uf = \mu \int f^2(r)U(r)dr$

(3.8.16)

From the relation between (3.8.10) and (3.8.16), we get

$$T - E = \mu \sigma_o^2$$

Noting that $\nu = \frac{E-E_o}{E_Q}$ and $\frac{\bar{h}^2}{2m} = Q = 1$, (3.8.17) becomes

$$T + \nu = \mu \sigma_o^2 \tag{3.8.18}$$

By using (3.7.29), (3.8.9.1) and (3.8.18) we obtain

$$\begin{aligned} b(\nu) &= (T+\nu)^2/\sigma_o^2 \\ &= (\mu \sigma_o^2)^2/\sigma_o^2 \\ &= \mu^2 \sigma_o^2 \end{aligned} \tag{3.8.19}$$

From (3.8.30) , (3.8.9.1), (3.8.15) and (3.8.18), we get

$$\begin{aligned} a(\nu) &= (T+\nu)^3 \sigma_1^3/(2\pi)^2 \sigma_o^7 \\ &= \frac{\mu^3 \sigma_o^6 \sigma_1^3}{(2\pi)^2 \sigma_o^7} \\ &= \frac{\mu^3 \sigma_1^3}{(2\pi)^2 \sigma_o} \end{aligned} \tag{3.8.20}$$

One can determine the function f(r) and μ by using (3.8.9) and (3.8.7). These functions can be solved self consistently by a computer. Then the values from (3.8.14), σ_o from (3.8.10) can be calculated. As a result the value $a(\nu)$, $b(\nu)$ can be obtained and the results is shown in Table 3.1. In order to study the behavior of the exponent of $\rho(\nu)$, one considers

$$n(\nu) = d\log b(\nu)/d\log\nu$$

$$= \frac{2}{b}\frac{db(\nu)}{d\nu} \qquad (3.8.21)$$

By using the dimensionless quantity $\xi = \xi/E_Q^2$, they plot the value of $n(\nu)$ versus $\xi = b(\nu)/_{10}$ as shown in Fig 3.1 where

$$\xi = \frac{8\pi e^4 (m\ )^2 \bar{N}}{\bar{h}^4 \ \ \varepsilon Q^5} \qquad (3.8.22)$$

This curves shows that $n(\nu)$ varies smoothly from $\frac{1}{2}$ to 2 as ν increases which is in agreement with the experimental value of the absorbtion spectrúm at the band tail states. (Halperin and Lax consider the validity region of $\rho(\nu)$ for screened Coulomb case and they conclude that when consider the states deep in the tail where the excited states at ν is quite small. The use of minimum counting method should valid). The limiting values of $a(\nu)$, $b(\nu)$, and $n(\nu)$ are shown in Table 3.1. The plotting of $\rho(\nu)$ and ν is shown in Fig. 3.2 when ξ has some values. The dimensionless $b(\nu)$ is shown in Fig 3.3

$\nu \ll 1$	$\nu \gg 1$
$a(\nu) \sim 0.4\,\nu^{3/2}$	$\sim 10^{-2}\,\nu^{7/2}$
$b(\nu) \sim 3\,\nu^{1/2}$	$\sim \nu^{2}$
$n(\nu) \sim \frac{1}{2}$	~ 2

Table 3.1 The limiting values of $a(\nu)$, $b(\nu)$ and $n(\nu)$.

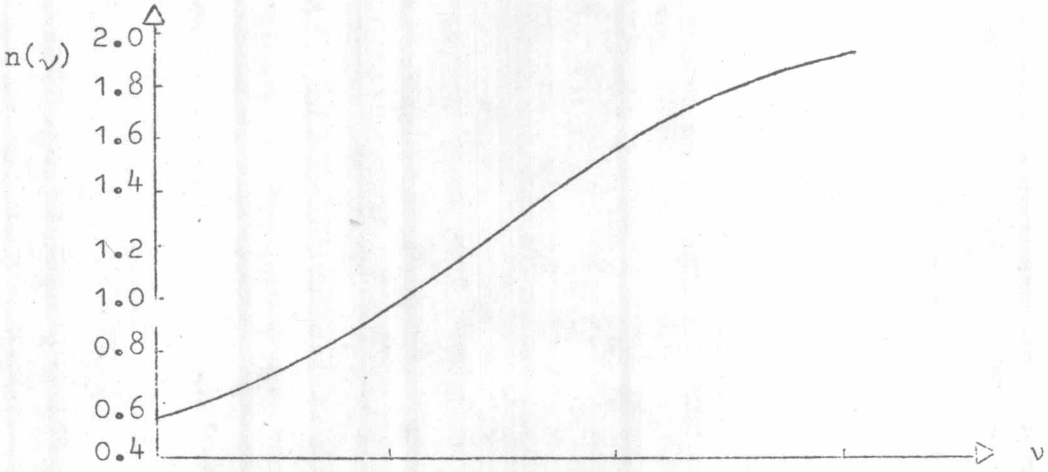

Fig 3.4 The logarithmic derivative $n(\nu) = d\log b(\nu)/d\log\nu$ of the $b(\nu)$ in the density of states.

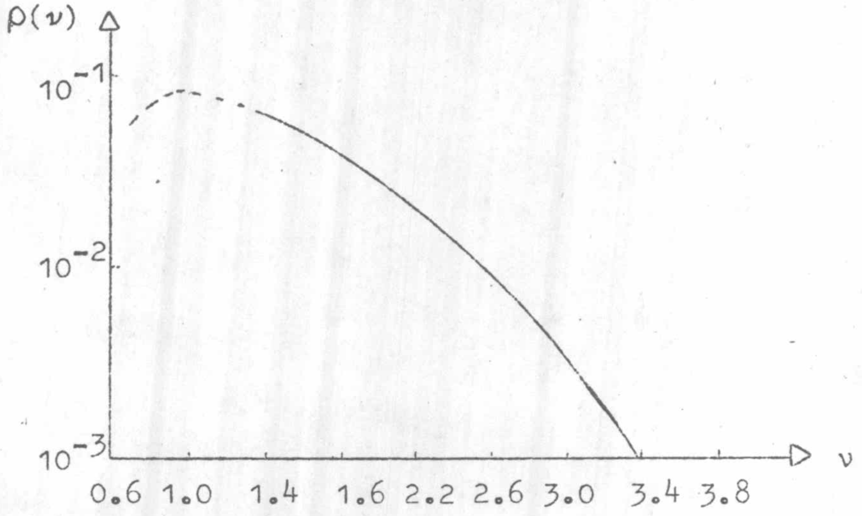

Fig 3.5 The density of states ρ in dimensionless form.

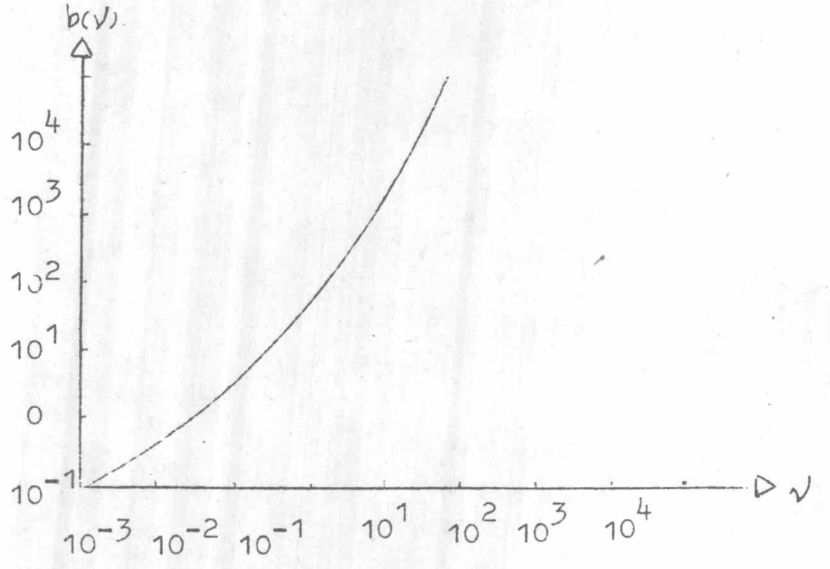

Fig 3.6 The function b(ν) obtained from the tabulated values of Halperin and Lax.