# CHAPTER II

# WAVE MECHANICS METHOD

หอสมุดกลาง สถาบันวิทยบริการ จุฬาลงกรณ์มหาวิทยาลัย

## 2.1 Introduction

Halperin and Lax[5] presented a theory which is based on Schrödinger formulation of quantum mechanics. Their theory can be used numerically to calculate the density of states in the low - energy tail of an electron band for a semiconductor containing of a high density of impurities. In one dimension, their theory reduces to the white noise model.

## 2.2 One - Dimensional Model

To understand the theory of Halperin and Lax, we first consider a model in which an electron is described by a Hamiltonian of the form

$$H = T + V(\vec{x}) . \qquad 2.2.1$$

The operator T is the " kinetic energy " of the particle with mass m, and is invariant under spatial translation. For one - band Hamiltonian, T has the simple form

$$T = -\frac{\hbar^2}{2m}\nabla^2 + E_o . \qquad 2.2.2$$

The constant $E_o$ is the average potential of N atoms. The potential $V(\vec{x})$ is the random potential of the atoms about the mean value, and it may be written in the form

$$V(\vec{x}) = \sum_{i=1}^{N} v(\vec{x} - \vec{z}_i) - E_o . \qquad 2.2.3$$

The quantity $v(\vec{x} - \vec{z}_i)$ is the potential at point $\vec{x}$ which due to a single atom at point $\vec{z}_i$

The density of states for the model is defined by

$$\rho(E) = \frac{1}{\Omega} < \sum_i \delta(E - E_i)> , \qquad 2.2.4$$

where $E_i$ is the energy of the i th eigenstate of the Hamiltonian H, $\Omega$ is the length of the array atoms in one dimension, and the angular bracket <> indicates an average over the atom positions.

## 2.3 First Order Approximation

The central assumption of Halperin and Lax is that all the eigenstates, at a given energy E in the low - energy tail, have the same shape. In other words, they assume that for all eigenstates $\psi_i$, such that $E_i \simeq E$, they have

$$\psi_i(\vec{x}) \simeq f(\vec{x} - \vec{x}_i) , \qquad 2.3.1$$

where f is a fixed function which depends on the parameter E. The point $\vec{x}_i$, the " center " of the i th wave function, will be different for each state. The wave function $\psi_i$ will be assumed to vary slowly from one lattice site to the next, and will be localized in the crystal in the vicinity of a potential well of the correct size to bind a wave function of the prescribed energy E. In the case of a high concentration of atoms, there will be many atoms within the range of the wave function $\psi_i$. Thus many atoms contribute to the potential well.

The function $f(\vec{x})$ must be assumed to be real, normalized, and unique. If the form of the function $f(\vec{x})$ is known for the given value of the energy E, the function $f(\vec{x} - \vec{y})$ can be used to define a variational energy $E_f(\vec{y})$, which is the matrix element of the Hamiltonian H in the states of $f(\vec{x} - \vec{y})$ :

$$E_f(\vec{y}) = \int d\vec{x} f(\vec{x} - \vec{y}) H f(\vec{x} - \vec{y}). \qquad 2.3.2$$

The variational energy is itself the sum of two terms

$$E_f(\vec{y}) = \Theta + V_s(\vec{y}), \qquad 2.3.3$$

where

$$\Theta = \int d\vec{x}\, f(\vec{x} - \vec{y}) T f(\vec{x} - \vec{y}), \qquad 2.3.4$$

$$V_s(\vec{y}) = \int d\vec{x}\, f(\vec{x} - \vec{y})^2 V(\vec{x}). \qquad 2.3.5$$

The kinetic - energy term $\Theta$ is independent of the choice of $\vec{y}$, whereas the potential term $V_s(\vec{y})$ is an average of the random potential $V(\vec{x})$ in a certain region centered about $\vec{y}$, and will depend on the choice of $\vec{y}$. The function $V_s(\vec{y})$ may be thought of as a smoothed version of the original potential and will exibit a large negative fluctuation in each region which binds a low - energy tail.

If (2.3.1) is assumed to hold, then the points $\vec{x}_i$ which are the centers of wave functions $\psi_i$ with $E_i \simeq E$ must satisfy

$$E_f(\vec{x}_i) \simeq E , \qquad 2.3.6$$

where the position $\vec{x}_i$ is a point such that $E_f(\vec{y})$ is a local minimum at $\vec{x}_i$. In other words, they define a local minimum as any point where $\vec{\nabla}E_f(\vec{y})$ equals zero, and the second derivatives are positive. Furthermore, the variational energy $E_f(\vec{y})$ is a ground-state energy of the local potential well, because potential wells strong enough to bind a wave function in the low - energy tail will be few and far between ; the probability of finding two overlapping wells, or of finding one isolated well so deep that we must consider the first excited state of the well, is negligibly small. One also finds that there will be only one local minimum in $E_f$ for each deep potential well and thus there will be a bound state $\psi_i$ at each local minimum satisfying (2.3.6).

If there is a one - to - one correspondence between local minimum in $E_f(\vec{y})$ and the energies in the vicinity of E, then the number of eigenstates with energy E is approximately equal to the number of local minima in $E_f(\vec{y})$ with value E. Thus (2.2.4) becomes

$$\rho_f(E) = \frac{1}{\Omega dE} \{\text{Number of local minima in } E_f(\vec{y}) \text{ such that at the minimum } E \leq E_f(\vec{y}) \leq E + dE.\} \qquad 2.3.7$$

The subscript f on the density of states remind that the validity of the estimate will depend on the correct choice of f.

Let $\{\vec{y}_i\}$ be the set of all points such that $E_f(\vec{y})$ is a local minimum at $\vec{y} = \vec{y}_i$. Then the density of states may be written as[5]

$$\rho_f(E) \equiv \langle \delta[E - E_f(\vec{y})] \sum_i \delta(\vec{y} - \vec{y}_i) \rangle . \qquad 2.3.8$$

The best choice of f is that which maximizes the value of $\rho_f(E)$. The fact that $E_f(\vec{x}_i)$ is equal to or larger than the true energy $E_i$ together with the fact that the density of states in the tail decreases rapidly with decreasing energy, implies that

$$\rho_f(E) \leq \rho(E) . \qquad 2.3.9$$

The equality sign in (2.3.9) would hold only if $E_f(\vec{y}) = E_i$ for all the wave functions with $E_i \approx E$, i.e., if assumption (2.3.1) were exact for the function f in equestion. Although (2.3.1) will not be exact, they get the best possible approximation to the true density of states by by choosing f maximize $\rho_f(E)$. Thus they make the approximation

$$\rho_1(E) \equiv \max_f \rho_f(E). \qquad 2.3.10$$

## 2.4 Gaussian Statistics

Halperin and Lax study in detail the case in which the random potential $V(\vec{x})$ obeys Gaussian statistics. The statistical properties of a set of Gaussian variables with mean zero are completely determined by the second moment of the distribution. The properties of $V(\vec{x})$ are thus determined by the autocorrelation function $\langle V(\vec{x})\, V(\vec{x}')\rangle$ . It is convenient to write

$$\langle V(\vec{x})V(\vec{x}')\rangle = \xi W(\vec{x} - \vec{x}'), \qquad 2.4.1$$

where the parameter $\xi$ is proportional to the concentration of atoms and to the square of the strength of the individual atoms, and where

the function $W(\vec{x} - \vec{x}')$ can be written in the form

$$W(\vec{x} - \vec{x}') = \int d\vec{z}_i v(\vec{x} - \vec{z}_i) v(\vec{x}' - \vec{z}_i). \qquad 2.4.2$$

The energy E will be in the low - energy tail if $E_o - E$ is large compared with the fluctuations in the smoothed potential $V_s(\vec{x})$, Thus the terms that are important for properties of the low - energy tail in a Gaussian potential are those which are important in the limit $\xi \to 0$, when the energy E is held fixed. Except for terms which are negligible in this limit, the approximate density of states $\rho_f$ in one dimension is

$$\rho_f(E) = \frac{\sigma_1(\theta - E)}{2\pi\xi\sigma_o^3} \exp\{-\frac{(\theta - E)^2}{2\xi\sigma_o^2}\} , \qquad 2.4.3$$

where

$$\sigma_o^2 = G(0) , \qquad 2.4.4$$

$$\sigma_1^2 = -G''(0) , \qquad 2.4.5$$

and

$$G(\vec{y} - \vec{y}') \equiv \iint d\vec{x}d\vec{x}' f^2(\vec{x} - \vec{y}) f^2(\vec{x}' - \vec{y}') W(\vec{x} - \vec{x}'). \qquad 2.4.6$$

In the low - energy tail, the important factor on the right -hand side of (2.4.3) is the exponential factor. When trying to find the function f which maximizes $\rho_f$, it suffices to use the function f which minimizes the expression

$$\Gamma(E,f) = (\theta - E)^2/\sigma_o^2 . \qquad 2.4.7$$

Application of variational calculus to (2.4.7), leads to a nonlinear differential equation for f of the form

$$(T + V_o)f = Ef, \qquad 2.4.8$$

with $V_o(\vec{x})$ itself is given by[9]

$$V_o(\vec{x}) = -\mu \int d\vec{x}' W(\vec{x} - \vec{x}')f(\vec{x}')^2. \qquad 2.4.9$$

In (2.4.9), $\mu$ is a Lagrange multiplier which is determined by the requirement that.

$$\int d\vec{x} f^2(\vec{x}) = 1 . \qquad 2.4.10$$

The value of $\mu$ is related to $\theta$ and $\sigma_o$ by

$$\mu = (\theta - E)^2 / \sigma_o^2. \qquad 2.4.11$$

The pair of (2.4.8) and (2.4.9) which they called the Hartree equation may be solved for $f(\vec{x})$ and $\mu$ by an analytic procedure only for the white noise potential in one dimension. For other case, these two equations must be solved by an iterative procedure. The approximate density of states $\rho_1(E)$ is obtained when this function f is used to evaluate the quantities $\theta$, $\sigma_o$, and $\sigma_1$, that appear in (2.4.3).

## 2.5 One - Dimensional White Noise Model

The white noise potential is characterized by Gaussian statistics, with the autocorrelation

$$\langle V(x)V(x')\rangle = \xi\delta(x - x'). \qquad 2.5.1$$

When the individual scattering potentials are written in the form[5]

$$v(x - z_i) = u\eta\delta(x - z_i), \qquad 2.5.2$$

then

$$\xi = \bar{N}\, u^2\eta^2 , \qquad 2.5.3$$

where the constant $\bar{N}$ is the concentration of atoms, the quantity $u\eta$ is used to correct the energy unit, and the parameter $\eta$ is the strength of the potential.

By choosing units where $\hbar$ and m are equal to unity, and by choosing the zero of energy such that $E_o = 0$. The kinetic energy is then given by

$$T = -\frac{1}{2}\frac{d^2}{dx^2} . \qquad 2.5.4$$

For the white noise model, the " Hartree equation," (2.4.8) and (2.4.9), takes the simple form

$$-\frac{1}{2} f''(x) - \frac{1}{2}\mu f(x)^3 = Ef(x). \qquad 2.5.5$$

However, (2.5.5) may be written

$$-\frac{1}{2}f''(x) - \frac{1}{2}\mu f(x)^3 = -\frac{1}{2}\kappa^2 f(x) , \qquad 2.5.6$$

where

$$-\frac{1}{2}\kappa^2 = E. \qquad 2.5.7$$

Multiplying by $f'(x)$ and integrating, we get

$$[f'(x)]^2 = \kappa^2 f(x)^2 - \frac{1}{2}\mu f(x)^4 + \text{constant}. \qquad 2.5.8$$

Since $f'(x) = f(x) = 0$ when $x = \infty$, the constant in (2.5.8) must equal zero. The origin will be chosen so that $f(0)$ is a maximum and hence, $f'(0) = 0$. Thus (2.5.8) implies

$$\frac{1}{2}\mu f(0)^2/\kappa^2 = 1. \qquad 2.5.9$$

If one defines

$$u(x) = f(\kappa^{-1}x) \,/\, f(0), \qquad 2.5.10$$

then one has $u(0) = 1$, and

$$u'(x) = -\left[u(x)^2 - u(x)^4\right]^{1/2} \quad \text{for } x \geqslant 0. \qquad 2.5.11$$

The sign of (2.5.11) is fixed by noting that $u(x)$ is a maximum at $x = 0$. From (2.5.11) it follows that, for $x \geqslant 0$,

$$x = \int_u^1 \frac{dv}{v(1-v^2)^{1/2}} = \tanh^{-1}\left[(1-u^2)^{1/2}\right] = \operatorname{sech}^{-1} u. \qquad 2.5.12$$

Similarly the procedure may be used for $x < 0$, and one finds that for all $x$,

$$u(x) = \operatorname{sech} x \,. \qquad 2.5.13$$

The normalization of $f(x)$ requires that

$$f(x) = \sqrt{\left(\frac{\kappa}{2}\right)}\operatorname{sech}\kappa x, \qquad 2.5.14$$

$$\mu = 4\kappa \,. \qquad 2.5.15$$

Finally the function f is used to evaluate the constant in(2.4.3). Thus Halperin and Lax find that

$$\rho_1(E) = \frac{1}{\sqrt{5}} \cdot \frac{4}{\pi} \cdot \frac{(-E)}{\xi} \cdot \exp\{-\frac{4\sqrt{2}}{3} \cdot \frac{\hbar}{\sqrt{m}} \cdot \frac{(-E)}{\xi}^{3/2}\}. \qquad 2.5.16$$

Comparing (2.5.16) with (1.5.1)

$$\rho_{as}(E) = \frac{4}{\pi} \cdot \frac{(-E)}{\xi} \cdot \exp\{-\frac{4\sqrt{2}}{3} \cdot \frac{\hbar}{\sqrt{m}} \cdot \frac{(-E)}{\xi}^{3/2}\}. \qquad 1.5.1$$

we find the agreement between $\rho_1$ and $\rho_{as}$ to be remarkably good. The power of E in the exponent and in front of the exponential are correct. The numerical factor in the exponent is exact, but infront of the exponential term is too small by a factor of $\sqrt{5}$ . However, the factor $1/\sqrt{5}$ will be removed if one includes the "average higher-order energy correction," described in the next section.

## 2.6 Second Order Approximation

Because the assumption that all the eigenstates at a given energy in the tail have the same shapes is not exact, the first order approximation leads to a small overestimate of the energy of each eigenstates, and an underestimate of the density of states. Halperin and Lax improve their first order approximation by including the effect of the "average higher - order energy correction." This correction changes the approximate density of states by displacing every energy calculated in their first order approximation by the expectation value of the energy correction due to the difference between the true

011722

Hamiltonian and the unperturbed Hamiltonian.

To find the energy correction, they expand the difference $E_i - E_f(\vec{x}_i)$ in powers of the perturbation $V(\vec{x}) - V_o(\vec{x}-\vec{x}_i)$. Halperin and Lax[9] write

$$E_i = E_f + \varepsilon_1 + \varepsilon_2 + \ldots, \tag{2.6.1}$$

where $\varepsilon_n$ is of order of $(V-V_o)^n$. The first term $\varepsilon_1 = 0$ for the condition that $E_f = E$. The second term $\varepsilon_2$ depends on the "modified Green's function $\hat{G}$" which is defined by

$$[E-T-V_o(\vec{x})]\hat{G}(\vec{x},\vec{x}') = \delta(\vec{x}-\vec{x}') - f(\vec{x})f(\vec{x}'). \tag{2.6.2}$$

If $\hat{G}$ is known, they can calculate the energy $\varepsilon_2$. They define the "average higher-order energy correction C(E)" by

$$-\xi C(E) = \lim_{\xi \to 0} \langle\langle \varepsilon_2 \rangle\rangle_E, \tag{2.6.3}$$

where the double angular brackets with subscript E indicates the conditional expectation value of the variable $\varepsilon_2$.

Halperin and Lax show that the corrected density of states $\rho_2(E)$ is related to C(E) by the following equation

$$\rho_2(E) = \exp\{\mu C(E)\}\, \rho_1(E), \tag{2.6.4}$$

where $\mu = 4\kappa$. The average higher - order energy correction C(E) has been evaluated, and was found to be

$$C(E) = \left(\frac{13}{72}\right)\kappa^{-1}. \qquad 2.6.5$$

It follows that

$$\rho_2(E) = \exp\left\{\frac{13}{18}\right\}\rho_1(E), \qquad 2.6.6$$

or, equivalently,

$$\rho_2(E) = \frac{e^{13/18}}{\sqrt{5}} \cdot \frac{4}{\pi} \cdot \frac{(-E)}{\xi} \cdot \exp\left\{\frac{-4\sqrt{2}}{3} \cdot \frac{\hbar}{\sqrt{m}} \cdot \frac{(-E)}{\xi}^{3/2}\right\}. \qquad 2.6.7$$

The factor $(1/\sqrt{5})\exp\{13/18\}$ equals to 0.921, and they were therefore able to reproduce the exact asymptotic value to within an error of less than 8 %.