QUANTUM THEORY OF IMPURITY-BAND TAILS

In Halperin and Lax theory[25,26], an impurity potential is considered only as screened Coulomb potential while in Sa-yakanit theory[27,29,32] both screened Coulomb potential and Gaussian potential are considered.

2.1 Halperin and Lax Theory (Minimum Counting Method)

Halperin and Lax have proposed a new theory, using the full quantum theory of Schrödinger for calculating the density of states $\rho(E)$ in the low energy-tail of an impurity band in heavily doped semiconductor based upon counting minima in an appropriately smoothes version of the random potential.

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2.1.1 Minimum Counting Method

In heavily doped semiconductor, there are many impurity atoms within a volume which characterize the "spread" or the "width" of a typical wave function. These impurities are distributed in a random manner throughout the solid. In the region of high impurity concentration the potential is deep, the wave function is narrow and the electron kinetic energy of localization is large. In the region of low

Concentration the potential is shallow, the wave function is spread out and the electron kinetic energy of localization is small. Halperin and Lax assume that the impurity potential distribution obeys Gaussian statistic. And they expect, therefore, that there will be the most probable shape for the wave function, not too narrow and not too spread out and assume that at a given energy E, in the low-energy tail, almost all of the wave function have approximately the same shape. For determining the probable shape of the wave function, Halperin and Lax assume that for a given energy E there is an optimum well depth to get the most value of low E_i, they denote the wave function $\psi_i(\vec{x})$ for the optimum well by

$$\psi_i(\vec{x}) \simeq f(\vec{x} - \vec{y}_i) \qquad (2.1.1)$$

where $f(\vec{x} - \vec{y}_i)$ is a fixed function for each energy E and $\vec{y}_i$ is a position variable which may be anywhere in the crystal and will be different for each eigenstate. In this case $f(\vec{x} - \vec{y}_i)$ is a real value function satisfying the normalization condition :

$$\int f^2(\vec{x} - \vec{y}_i)\, d\vec{x} = 1 \qquad (2.1.2)$$

Since the Hamiltonian of the disordered solid is given by

$$H = T + V(\vec{x}) \qquad (2.1.3)$$

where $\quad$ T $\quad = \quad -\hbar^2 \nabla^2/2m^* + E_O$ $\qquad$ (2.1.4)

$V(\vec{x})$ is the random potential due to the impurity atoms and E_O is the energy of the unperturbed parabolic band edge.

According to the quantum-mechanical theory there is the correspondence between the wavefunction and the eigen energy E for each state. Then, the associated energy for a trial wave function $f(\vec{x} - \vec{y}_i)$ is

$$E(\vec{y}_i) \quad = \quad \int f(\vec{x} - \vec{y}_i) \, H \, f(\vec{x} - \vec{y}_i) \, d\vec{x} \qquad (2.1.5)$$

Substituting for the value of H from (2.1.3) and (2.1.4) one gets

$$E(\vec{y}_i) \quad = \quad \int f(\vec{x} - \vec{y}_i)(-\hbar^2\nabla^2/2m^*) \, f(\vec{x} - \vec{y}_i) \, d\vec{x}$$

$$+ \, E_O + \int f^2(\vec{x} - \vec{y}_i) \, V(\vec{x}) \, d\vec{x} \qquad (2.1.6)$$

$$= \quad T_s + E_O + V_s(\vec{y}_i) \quad \equiv \quad \theta + V_s(\vec{y}_i) \qquad (2.1.7)$$

Note that the kinetic energy θ is independent to the choice of $\vec{y}_i$, because the operator T is translationally invariant. The potential energy $V_s(\vec{y}_i)$ is an average of the potential $V(\vec{x})$ in a region about $\vec{x} = \vec{y}_i$. As $\vec{y}_i$ is permitted to vary throughout the crystal, $V_s(\vec{y}_i)$ will fluctuate about an average value of zero, and at various places in the crystal $V_s(\vec{y}_i)$ will exhibit an unusual large negative fluctuation.

These places correspond to regions of very low $V(\vec{x})$, and hence to the places expected to find a low-energy eigenstate $\psi_i(\vec{x})$. Since a variational approximation of the ground-state energy of a system always overestimates this energy. Hence, one expects that $E(\vec{y}_i)$ in region of negative fluctuations will always be larger than the true energy E_i of the local low-energy eigenstate. The best estimation of the energy E_i is thus obtained by choosing $\vec{y}_i$ so that $E(\vec{y}_i)$ is as small as possible, i.e., so that $E(\vec{y}_i)$ is a local minimum. Halperin and Lax assume that there is a chose one-to-one correspondence between local minima in $E(\vec{y}_i)$ 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 $E(\vec{y}_i)$ with value E. For example in Fig. 2.1 there is only one local minima not three with the energy E_i. Thus one has the following approximation to the density of states in the volume Ω

$$\rho_f(E) = \frac{1}{\Omega} \, dE \, \Big[\text{Number of local minima in } E(\vec{y}_i) \text{ such that}$$

$$\text{at the minimum } E \leqslant E(\vec{y}_i) \leqslant E + dE \Big] \quad (2.1.8)$$

Halperin and Lax define "a local minima" as any point where $\nabla E(\vec{y}_i) = 0$ and the second derivatives are positive. Since only $V_s(\vec{y}_i)$ in (2.1.7) depend on $\vec{y}_i$, then $\nabla E(\vec{y}_i) = 0$ can be replaced by $\nabla V_s(\vec{V}_i) = 0$.
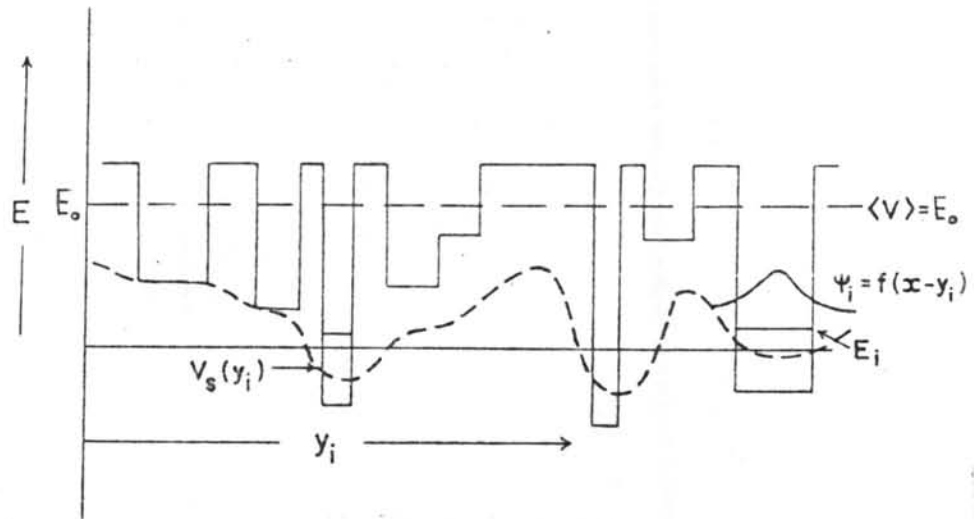
Fig. 2.1 Potential wells in heavily doped semiconductor.

2.1.2 Density of states

The density of states is defined by

$$\rho(E) \quad = \quad \frac{1}{\Omega} \; < \sum_i \; \delta(E - E_i) \; >_V \tag{2.1.9}$$

with the assumption that all E_i are given by the optimum $E(\vec{y}_i)$.

$$E_i \quad \simeq \quad E(\vec{y}_i) \quad = \quad \theta + V_s(\vec{y}_i) \tag{2.1.10}$$

Hence

$$\rho_f(E) \quad = \quad \frac{1}{\Omega} \left\langle \sum_i \delta\left[E - (\theta + V_s(\vec{y}_i))\right] \right\rangle_V \qquad (2.1.11)$$

when the property of the Dirac delta function $\int_{-\infty}^{\infty} f(x)\, \delta(x-a)\, dx = f(a)$
is applied the density of states becomes

$$\rho_f(E) \quad = \quad \int \frac{d\vec{y}}{\Omega} \left\langle \sum_i \delta(\vec{y}-\vec{y}_i)\, \delta\left[E-\theta-V_s(y)\right] \right\rangle_V \qquad (2.1.12)$$

where $\left\{\vec{y}_i\right\}$ is the set of all points satisfying $\nabla V_s(\vec{y}_i) = 0$.
After averaging, the quantity in brackets in (2.1.12) becomes
independent of $\vec{y}$, and the integration over $\vec{y}$ merely yields a factor
of Ω . Thus it may be written as

$$\rho_f(E) \quad = \quad \left\langle \sum_i \delta(\vec{y}-\vec{y}_i)\, \delta\left[E-\theta-V_s(\vec{y})\right] \right\rangle_V \qquad (2.1.13)$$

Next make a transformation from the variable $\vec{y}$ to $\nabla V_s(\vec{y})$ by
writing

$$\sum_i \delta(\vec{y}-\vec{y}_i) \quad = \quad \delta\left[\nabla V_s(\vec{y})\right] \left|\det \quad \nabla\nabla V_s(\vec{y})\right| \qquad (2.1.14)$$

The determinant of the second derivatives in (2.1.14) arises as the
Jacobian of the transformation. Equation (2.1.13) can now be
written :

$$\rho_f(E) \quad = \quad p(\lambda) \; p_3(\Lambda \mid \lambda) \; \chi(\lambda, \Lambda) \tag{2.1.16}$$

where the function $p(\lambda)$ is the probability density for $V_s(\vec{y})$ to take on the value λ at an arbitrary point $\vec{y}$. $P_3(\Lambda \mid \lambda)$ is the conditional probability density for $\nabla V_s(\vec{y})$ to take on the value Λ, when it is specified that $V_s(\vec{y}) = \lambda$, and $\chi(\lambda, \Lambda)$ is the conditional expectation value of $|\det \; \nabla\nabla \; V_s(\vec{y})|$, when it is specified that $V_s(\vec{y}) = \lambda$ and $\nabla V_s(\vec{y}) = \Lambda$. Halperin and Lax are interested in the functions p, p_3 and χ when $\lambda = E - \theta$ and $\Lambda = 0$.

To estimate the probability function it is needed to know the two-point autocorrelation function $\langle V_s(\vec{y}) \, V_s(\vec{y}') \rangle$. This function may be expressed in terms of autocorrelation function $\langle V(\vec{x}) V(\vec{x}') \rangle$ of the original potential, $v(\vec{x} - \vec{z})$.

$$\langle V_s(\vec{y}) V_s(\vec{y}') \rangle \quad = \quad \int f^2(\vec{x}-\vec{y}) \; f^2(\vec{x}'-\vec{y}') \langle V(\vec{x}) V(\vec{x}') \rangle \; d\vec{x} \; d\vec{x}' \tag{2.1.17}$$

and

$$\langle V(\vec{x}) V(\vec{x}') \rangle \quad = \quad \eta^2 \bar{N} \int v(\vec{x}-\vec{z}) \; v(\vec{x}'-\vec{z}') \; d\vec{z} \tag{2.1.18}$$

In order to exhibit explicity the dependence of these moments on the concentration of impurities $\bar{N}$ and the strength of the potential η^2. Halperin and Lax introduce a parameter

$$\xi \quad = \quad n^2 \bar{N} \tag{2.1.19}$$

Then (2.1.17) and (2.1.18) can be written as

$$\langle V_s(\vec{y}) \, V_s(\vec{y}\,') \rangle \quad = \quad \xi G(\vec{y} - \vec{y}\,') \tag{2.1.20}$$

$$\langle V(\vec{x}) \, V(\vec{x}\,') \rangle \quad = \quad \xi \, W(\vec{x} - \vec{x}\,') \tag{2.1.21}$$

where

$$G(\vec{y} - \vec{y}\,') \quad = \quad \int f^2(\vec{x} - \vec{y}) \, f^2(\vec{x}\,' - \vec{y}\,') \, W(\vec{x} - \vec{x}\,') \, d\vec{x} d\vec{x}\,' \tag{2.1.22}$$

and

$$W(\vec{x} - \vec{x}\,') \quad = \quad \int v(\vec{x} - \vec{z}) v(\vec{x}\,' - \vec{z}\,') d\vec{z} \tag{2.1.23}$$

when the concentration of impurities is sufficiently high, Halperin and Lax assume that Gaussian statistics can be used. The statistical properties of $V_s(\vec{y})$, in the Gaussian case, are completely determined by the two-point autocorrelation function $\langle V_s(\vec{y}) V_s(\vec{y}\,') \rangle$. Then, the function $p(\lambda)$ in (2.1.16) is a Gaussian distribution.

$$p(\lambda) \quad = \quad (2\pi\xi\sigma_o^2)^{-\frac{1}{2}} \exp(-\lambda^2/2\xi\sigma_o^2) \tag{2.1.24}$$

with variance

$$\xi\sigma_o^2 \quad \equiv \quad \langle \, V_s(\vec{y})^2 \, \rangle \quad = \quad \xi G(0) \tag{2.1.25}$$

For determining the conditional probability density for $\nabla V_s(\vec{y})$, $P_3(\lambda \mid \lambda)$, the covariance of $V_s(\vec{y})$ with its first derivative is considered. Such that

$$\langle \, V_s(\vec{y}) \, \nabla V_s(\vec{y}) \, \rangle \quad = \quad \xi \vec{\nabla}_{\vec{y}}{}' \, G(\vec{y} - \vec{y}{}') \, \Big|_{\vec{y}{}'=\vec{y}} \tag{2.1.26}$$

Because the function G, by definition, is an even function of its argument. Then

$$\langle \, V_s(\vec{y}) \, \nabla V_s(\vec{y}) \, \rangle = \quad 0 \tag{2.1.27}$$

This means that autocorrelated variables such as $V_s(\vec{y})$ and $\nabla V_s(\vec{y})$ are statistically independent. Thus $P_3(\lambda \mid \lambda)$ is independent of λ and reduces to the ordinary probability distribution of $\nabla V_s(\vec{y})$.

The covariances of the derivatives among themselves are given by

$$\langle \, [\nabla V_s(\vec{y})][\nabla V_s(\vec{y})] \, \rangle \quad = \quad - \, \xi \, \nabla \nabla \, G(0) \tag{2.1.28}$$

It is convenient to choose the coordinate axes such that the matrix of second derivatives of G is diagonal, with the form

$$\nabla\nabla G(0) \quad = \quad - \begin{vmatrix} \sigma_1^2 & 0 & 0 \\ 0 & \sigma_2^2 & 0 \\ 0 & 0 & \sigma_3^2 \end{vmatrix} \qquad (2.1.29)$$

Here, the three components of $\nabla V_s(\vec{y})$ are uncorrelated, and the function $P_3(\Lambda \mid \lambda)$ is simply the product of three Gaussians.

$$P_3(\Lambda \mid \lambda) \quad = \quad (2\pi\xi)^{-3/2} (\sigma_1\sigma_2\sigma_3)^{-1} \exp\left[-\frac{\Lambda_1^2}{2\xi\sigma_1^2} - \frac{\Lambda_2^2}{2\xi\sigma_2^2} - \frac{\Lambda_3^2}{2\xi\sigma_3^2} \right]$$

$$(2.1.30)$$

Since $\Lambda = 0$ (2.1.30) becomes

$$P_3(0 \mid \lambda) \quad = \quad (2\pi\xi)^{-3/2} (\sigma_1\sigma_2\sigma_3)^{-1} \qquad (2.1.31)$$

To find $\chi(\lambda, \Lambda)$, the conditional expectation value of the determinant of the second derivatives of $V_s(\vec{y})$, it can be written as

$$\nabla\nabla V_s(\vec{y}) \quad = \quad V_s(\vec{y})\vec{M} + \vec{X} \qquad (2.1.32)$$

where $\vec{M}$ is a constant matrix, and $\vec{X}$ is a matrix of variables,

uncorrelated with $V_s(\vec{y})$, which have mean zero and variances proportional to ξ . The matrix $\vec{M}$ is given by

$$\vec{M} = \frac{\langle V_s(\vec{y}) \nabla\nabla V_s(\vec{y}) \rangle}{\langle V_s(\vec{y})^2 \rangle} = \frac{\nabla\nabla G(0)}{G(0)} \qquad (2.1.33)$$

By using the condition $V(\vec{y}) = \lambda$ and variance $V_s(\vec{y}) = \xi\sigma_o^2 = \xi G(0)$ one obtains

$$\vec{M} = \frac{(\theta-E)^3 \sigma_1^2 \sigma_2^2 \sigma_3^2}{\sigma_o^6} = \chi(E-\theta, \ 0) \qquad (2.1.34)$$

Combining the results for P, P_3, and χ , when $\lambda = E-\theta$ and $\Lambda = 0$, the density of states obtained is

$$\rho_f(E) = (2\pi\xi\sigma_o^2)^{-\frac{1}{2}} \exp\left[-(\theta-E)^2/2\xi\sigma_o^2\right] (2\pi\xi)^{-3/2} (\sigma_1\sigma_2\sigma_3)^{-1}$$

$$\times (\theta-E)^3 \sigma_1^2 \sigma_2^2 \sigma_3^2 / \sigma_o^6 \qquad (2.1.35)$$

$$\rho_f(E) = \frac{(\sigma_1\sigma_2\sigma_3)(\theta-E)^3}{(2\pi\xi)^2 \sigma_o^7} \exp\left[-(\theta-E)^2/2\xi\sigma_o^2\right] \qquad (2.1.36)$$

Now consider the problem of finding the best choice of $f(\vec{x} - \vec{y}_i)$. In the spirit of the variational calculation, it is known

that $f(\vec{x} - \vec{y}_i)$ gives a higher energy than the true eigenvalue. The density of states is expected to decrease rapidly and monotonically in the tail, any density of states calculated will be smaller than the true value. Therefore, for finding the best choice of the wave function $f(\vec{x} - \vec{y}_i)$, Halperin and Lax maximize the density of state $\rho_f(E)$. When $\xi \longrightarrow 0$, $\rho_f(E)$ is dominated by the exponential factor. The further approximation is done by maximizing the exponential factor in (2.1.36) or equivalently, to minimize the expression

$$\Gamma \equiv \frac{(\theta - E)^2}{\sigma_o^2} = \frac{\left[E - \int f(\vec{x}) T f(\vec{x}) d\vec{x} \right]^2}{\int f^2(\vec{x}) f^2(\vec{x}) W(\vec{x} - \vec{x}') d\vec{x} d\vec{x}'} \tag{2.1.37}$$

Let

$$\rho_1(E) = \max_f \left[\rho_f(E) \right] \tag{2.1.38}$$

So that

$$\rho_1(E) = A(E) \, \xi^{-2} \, \exp \left[-B(E)/2\xi \right] \tag{2.1.39}$$

where $A(E)$ is the pre-factor of $\rho_f(E)$ and $B(E)$ is the minimum value of Γ

$$A(E) = \frac{\sigma_1 \sigma_2 \sigma_3 \, (\theta - E)^3}{(2\pi)^2 \, \sigma_o^7} \tag{2.1.40}$$

$$B(E) = \Gamma_{min} = \min \left[(\theta - E)^2 / \sigma_o^2 \right] \tag{2.1.41}$$

and

$$\Gamma_{min} \equiv \frac{\partial}{\partial f} \left[\frac{\theta - E}{\sigma_0} \right]^2 = 0$$

Γ_{min} is determined by the ratio method, the method of variational calculation, suggested by Butkov[33]. This leads to the Hartree-Fock like equation for $f(\vec{x})$

$$T f(\vec{x}) - \mu f(\vec{x}) \int f^2(\vec{x}') W(\vec{x} - \vec{x}') \, d\vec{x}' = E f(\vec{x}) \tag{2.1.42}$$

or

$$T f(\vec{x}) - \mu f(\vec{x}) \, U(\vec{x}) = E f(\vec{x}) \tag{2.1.43}$$

where μ is a lagrange multiplier, and

$$U(\vec{x}) = \int \left[f(\vec{x}') \right]^2 W(\vec{x} - \vec{x}') d\vec{x}' \tag{2.1.44}$$

Then multiply each side of (2.1.43) by $f(\vec{x})$ and integrate throughout the configuration space of the system, one obtains

$$\int f(\vec{x}) T \, f(\vec{x}) d\vec{x} - \mu \int \left[f(\vec{x}) \right]^2 U(\vec{x}) d\vec{x} = E \tag{2.1.45}$$

or

$$\theta - \mu \, \sigma_0^2 = E \tag{2.1.46}$$

$$(\theta - E) = \mu \sigma_0^2 \tag{2.1.47}$$

where

$$\theta \quad = \quad \int f(\vec{x}) \, T f(\vec{x}) \, d\vec{x} \tag{2.1.48}$$

and

$$\sigma_o^2 \quad = \quad \int \left[f(\vec{x}) \right]^2 U(\vec{x}) \, d\vec{x} \tag{2.1.49}$$

Similary   using (2.1.22), (2.1.29), and (2.1.43) , one gets

$$\sigma_1^2 \quad = \quad - \frac{1}{3} \int U(\vec{x}) \, \nabla^2 \left[f(\vec{x}) \right]^2 \, d\vec{x} \tag{2.1.50}$$

Then the numerical values of σ_o , σ_1, σ_2, σ_3 and the mean kinetic energy θ are substituted into (2.1.36) to get the density of states.

2.1.3 Screened Coulomb Potential

Halperin and Lax assume that an impurity potential having the screened Coulomb form

$$v(\vec{x} - \vec{z}) \quad = \quad \frac{- Ze^2}{\varepsilon_o |\vec{x}-\vec{z}|} \exp \ (-Q \, |\vec{x} - \vec{z}| \,) \tag{2.1.51}$$

where e is the electronic charge, ε_o is the dielectric constant of

the pure semiconductor, Q is the reciprocal screening length, and Ze is the charge of impurities. The autocorrelation function for the potential fluctuations can be evaluated by working with the Fourier transform of (2.1.23). The random position z can be integrated out. One finds after straightforward calculation that

$$W(\vec{x} - \vec{x}') \quad = \quad \xi \exp (-Q|\vec{x} - \vec{x}'|) \tag{2.1.52}$$

where

$$\xi \quad = \quad \frac{2\pi e^4 z^2}{Q\epsilon_o^2} \tag{2.1.53}$$

They also assume that the optimum choice of $f(\vec{x})$ is a spherically symmetric function. Let

$$f(\vec{x}) \quad = \quad (4\pi)^{-\frac{1}{2}} \; S(r)/r \tag{2.1.54}$$

where $r = |\vec{x}|$, and $S(r)$ is required to vanish at $r = 0$ and $r = \infty$. Substituting for the value of $f(\vec{x})$ and Ψ into the Hartree-Fock like eigenvalue equation, i.e (2.1.43) will result

$$\left[- \frac{\hbar^2}{2m^*} \frac{d^2}{dr^2} - \mu U(r) \right] S(r) \quad = \quad (E - E_o) S(r) \tag{2.1.55}$$

where $\quad U(r) \quad = \quad \int K(r, r') S(r')^2 dr' \tag{2.1.56}$

The averaging of the function $\exp(-Q |\vec{x} - \vec{x}'|)$ with respect to the angular coordinates of the variable $\vec{x}$ gives

$$K(r, r') \equiv \frac{1}{2} \int_{-1}^{1} \exp\left[-Q(r^2+r'^2+2rr'\mu)^{\frac{1}{2}}\right] d\mu \qquad (2.1.57)$$

Using the change of variable $R = (r^2 + r'^2 + 2rr'\mu)^{\frac{1}{2}}$

$$= r_> (1 + \frac{r_<^2}{r_>^2} + \frac{2r_< \mu}{r_>})^{\frac{1}{2}} \qquad \text{the above integral becomes}$$

$$K(r, r') = \frac{1}{2rr'} \int_{r_>-r_<}^{r_>+r_<} R \exp(-QR) dR \qquad (2.1.58)$$

By application of the formula $\int xe^{-Qx} dx = -e^{-Qx}(\frac{x}{Q} + \frac{1}{Q^2})$ $K(r,r')$ obtained is as:

$$K(r, r') = \frac{1}{Qrr'} e^{-Qr_>} \left[(r_> + Q^{-1}) \sin hQ \, r_< - r_< \cos hQr_< \right] \qquad (2.1.59)$$

where $r_>$ and $r_<$ are the greater and lesser, respectively, of the two numbers r' and r.

For simplicity, Halperin and Lax consider the whole calculations in unit of $E_Q = \hbar^2 Q^2/(2m^*) = 1$, then (2.1.55) reduces to

$$\left[-d^2/dr^2 - u\, U(r) \right] S(r) = -\nu\, S(r) \qquad (2.1.60)$$

where ν is the dimensionless energy,

$$\nu \equiv (E_0 - E)/E_Q \qquad (2.1.61)$$

and the density of states $\rho_1(E)$ in (2.1.39) can be rewritten as

$$\rho_1(E) = (E_\varrho^3 \varrho^3/\xi^2)\,a(\nu)\,\exp\left[-(E_\varrho^2/2\xi)b(\nu)\right] \qquad (2.1.62)$$

where $a(\nu)$ and $b(\nu)$, the universal dimensionless functions, are equal to $A(E)$ and $B(E)$ in units where $\varrho = \hbar^2/2m^* = 1$, i.e.

$$a(\nu) = A(E) = \frac{\sigma_1\sigma_2\sigma_3\,(\theta - E)^3}{(2\pi)^2\,\sigma_o^7} \qquad (2.1.63)$$

Since $f(\vec{x})$ is spherically symmetric, then $\sigma_1^2 = \sigma_2^2 = \sigma_3^2$ and using (2.1.47), one gets

$$a(\nu) = \frac{\sigma_1^3\,(\mu\,\sigma_o^2)^3}{(2\pi)^2\,\sigma_o^7} = \frac{\sigma_1^3\,\mu^3}{(2\pi)^2\,\sigma_o} \qquad (2.1.64)$$

From, (2.1.49) and (2.1.50) σ_o^2 and σ_1^2 can be written in the form of the radial wavefunction $S(r)$ as

$$\sigma_o^2 = \int_o^\infty \left[S(r)\right]^2 U(r)\,dr \qquad (2.1.65)$$

and

$$\sigma_1^2 = -\frac{1}{3}\int_o^\infty rU(r)\,dr\left[S(r)^2/r\right]'' \qquad (2.1.66)$$

The symbol $\left[\right]''$ denotes the second derivative d^2/dr^2.

Similarly, $\qquad b(\nu) \quad = \quad \mu^2 \sigma_o^2$ $\qquad\qquad$ (2.1.66)

and the logarithmic derivative $n(\nu)$ of the exponent $b(\nu)$ in $\rho_1 (E($ is

$$n(\nu) \quad \equiv \quad d \log b(\nu)/d \log \nu \qquad\qquad (2.1.67)$$

For each value of ν , Halperin and Lax solve (2.1.60) and (2.1.56) by using iteration process, i.e. a trial function is first used for $S(r)$ and the value of μ is varied until the solution $S(r)$ of (2.1.60) satisfies the required boundary conditions and the function $S(r)$ thus obtained is used as a new trial function in (2.1.56). The wave function finally obtained is used to calculate the constant $T = \theta - E_o = \mu\sigma_o^2 - \nu$, σ_o and σ_1 , and the function $a(\nu)$ and $b(\nu)$ of (2.1.62).

The limiting values of $a(\nu)$, $b(\nu)$ and $n(\nu)$ are shown in Table 2.1

Table 2.1 The limiting values of $a(\nu)$, $b(\nu)$ and $n(\nu)$ when a screened Coulomb potential is applied.

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

2.2 Sa-yakanit Theory

Sa-yakanit[27,29] presented a new theory, for calculating the density of states in heavily doped semiconductors using the path integral method of Feynman[30]. His theory succeeded in evaluating an expression for $\rho(E)$ which valid at all energies E[32]. Here one focuses on the density of states $\rho(E)$ in the deep tail state, which can be compared with Halperin and Lax theory[25,26], and consider the two different impurity potentials; the Gaussian potential and the screened Coulomb potential. The outline of Sa-yakanit theory is briefly mention as follow

2.2.1 Density of states

To calculate the density of states, the full expression (2.1.9) for $\rho(E)$ is started

$$\rho(E) \quad = \quad \frac{1}{\Omega} \quad < \sum_i \delta(E - E_i) >_V \qquad (2.2.1)$$

Next the retarded propagator $G(\vec{x}_2, \vec{x}_1, t)$ is introduced which describes the propagation of an electron from point $\vec{x}_1$ to $\vec{x}_2$. This propagator $G(\vec{x}_2, \vec{x}_1, t)$ is $(-i\hbar)$ times of the usual retarded Green's function and can be written as a path integral over all the possible paths between $\vec{x}_1$ and $\vec{x}_2$,

$$G(\vec{x}_2, \vec{x}_1, t) \quad = \quad \int D(\vec{x}(\tau)) \exp[(i/\hbar) S_e] \qquad (2.2.2)$$

where $D(\vec{x}(\tau))$ denotes the path-integral with boundary condition $\vec{x}(0) = \vec{x}_1$ and $\vec{x}(t) = \vec{x}_2$, S_e is the action

$$S_e = \int_0^t d\tau \left[\frac{m}{2} \dot{\vec{x}}^2(\tau) - V(\vec{x}(\tau)) \right] \qquad (2.2.3)$$

and $V(\vec{x}(\tau))$ denotes the sum of the impurity potentials,

$$V(\vec{x}(\tau)) = \sum_i v(\vec{x}(\tau) - R_i) \qquad (2.2.4)$$

where $v(\vec{x}(\tau) - R_i)$ represents the potential at $\vec{x}(\tau)$ due to an impurity at point R_i. The properties of the system are obtained from the averaging of $G(\vec{x}_2, \vec{x}_1, t)$ over all impurity configuration $\{R_i\}$. In the limits of weak impurity potential $v(\vec{x}(\tau)) - R_i) \longrightarrow 0$ and their high density $\bar{N} \longrightarrow \infty$ so that $\bar{N}v^2$ remains finite. The average propagator can be expressed in the forms

$$\bar{G}(\vec{x}_2, \vec{x}_1, t) = \langle G(\vec{x}_2, \vec{x}_1, t) \rangle_V = \int D(\vec{x}(\tau)) \, e^{(i/\hbar)S} \qquad (2.2.5)$$

where S is the full action of the random system given as

$$S = \int_0^t d\tau \left[\frac{m}{2} \dot{\vec{x}}^2(\tau) - \int_0^t d\tau E_0 + \frac{i}{2\hbar} \bar{N}\eta^2 \int_0^t \int_0^t d\tau d\sigma \, w(\vec{x}(\tau) - \vec{x}(\sigma)) \right] \quad (2.2.6)$$

Here the mean potential is taken to be E_0 and the autocorrelation function is defined by

$$w(\vec{x}(\tau) - \vec{x}(\sigma)) \quad = \int d\vec{R} \; v(\vec{x}(\tau) - \vec{R}) \; v(\vec{x}(\sigma) - \vec{R}) \tag{2.2.7}$$

The quantity η in (2.2.6) is parameter which one has introduced in order to discuss more easily the behavior of the density of states as a function of the strength of the impurity potential. The density of states per unit volume is then related to the diagonal part of the average propagator

$$\rho(E) \quad = \quad \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \bar{G}(0,0,t) \; \exp\left[(i/\hbar)Et \right] \tag{2.2.8}$$

To obtain the density of states expression, the approximate expression $\bar{G}$ in (2.2.5) have to be calculated. The path integral of the action S given in (2.2.6) is very difficult to evaluate analytically because it is not quadratic in $\vec{x}$ (only quadratic action will lead to integral path integration). To perform the path integral in (2.2.3), Sa-yakanit assumes that there will be an action which is simple, integrable and intimated the action S. He modelled the full action S by a non-local harmonic "trial" action

$$S_0 \quad = \int_0^t d\tau \; \frac{m}{2} \left[\dot{\vec{x}}^2(\tau) - \frac{\omega^2}{2t} \int_0^t d\sigma \, | \, \vec{x}(\tau) - \vec{x}(\sigma) \, |^2 \right] \tag{2.2.9}$$

where ω is an unknown parameter to be determined. Once the trial action S_0 has been introduced, one may proceed to find the average

propagator which can be written as

$$\bar{G}(0,0,t) \;=\; \bar{G}_o(0,0,t) \; \langle \exp\left[\,(i/\hbar)(S-S_o)\,\right]\rangle S_o \qquad (2.2.10)$$

where $\; G_o(0,0,t) \;=\; \int D(\vec{x}(\tau)) \; \exp\left[\,(i/\hbar)S_o\right] \qquad (2.2.11)$

and the symbol $\; \langle \,-----\,\rangle_{S_o} \;$ means averaging with respect to the trial action S_o

$$\langle\, \dot{F}\, \rangle_{S_o} \;=\; \frac{\int D(\vec{x}(\tau))\; F(\vec{x}(\tau))\, \exp\left[\,(i/\hbar)S_o\right]}{\int D(x(\tau))\; \exp\left[\,(i/\hbar)S_o\right]}$$

The approximation of (2.2.8) by the first cumulant results

$$\bar{G}_1(0,0,t) \;=\; \bar{G}_o(0,0,t)\; \exp\left[\,(i/\hbar)\,\langle\, S - S_o\, \rangle_{S_o}\,\right] \qquad (2.2.12)$$

Sa-yakanit finds that the diagonal part of the zeroth-order propagator $\bar{G}(0,0,t)$ can be calculated exactly as follows

$$\bar{G}_o(0,0,t) \;=\; \left(\frac{m}{2\pi i\hbar t}\right)^{3/2} \left(\frac{\omega t}{2\sin(\frac{1}{2}\omega t)}\right)^3$$

Then

$$\bar{G}_1(0,0,t) \;=\; \left(\frac{m}{2\pi i\hbar t}\right)^{3/2} \left(\frac{\omega t}{2\sin(\frac{1}{2}\omega t)}\right)^3 \exp\left[\,(i/\hbar)\,\langle\, S-S_o\, \rangle_{S_o}\,\right] \qquad (2.2.13)$$

Note that if the impurity potential is known, the density of states can be evaluated.

2.2.2 Gaussian potential

For an impurity potential having the Gaussian form

$$v(\vec{x}(\tau) - \vec{R}) = u^2(\pi \ell^2)^{-3/2} \exp\left[-|\vec{x}(\tau) - \vec{R}|^2/\ell^2\right] \qquad (2.2.14)$$

It follows from (2.2.7) that

$$w(\vec{x}(\tau) - \vec{x}(\sigma)) = u^2(\pi L^2)^{-3/2} \exp\left[-|\vec{x}(\tau) - \vec{x}(\sigma)|^2/L^2\right] \qquad (2.2.15)$$

where $L^2 = 2\ell^2$ denotes the autocorrelation length and u is another parameter introduced in order to take care the dimension of the system. After substitute the above equation into (2.2.6) S becomes

$$S = \int_0^t d\tau\, \frac{m}{2}\dot{\vec{x}}^2(\tau) - \int_0^t d\tau E_0 + \frac{i}{2\hbar}\xi_L \int_0^t\int_0^t d\tau d\sigma \exp\left[-|\vec{x}(\tau) - \vec{x}(\sigma)|^2/L^2\right] \quad (2.2.16)$$

where $\xi_L = \bar{N}\eta^2 u^2/(\pi L^2)^{3/2}$ has the dimension of the energy square. Sa-yakanit determines the average $\langle S-S_0\rangle_{S_0}$ for the case of a Gaussian potential which can be written as

$$\langle S-S_0\rangle_{S_0} = -E_0 t + \frac{i}{2\hbar}\xi_L(\frac{L^2}{4})^{3/2} t \int_0^t dx\, [j_L(x)]^{-3/2} - \frac{3}{2} i\hbar(\frac{\omega t}{2} \cot \frac{\omega t}{2} - 1)$$

$$(2.2.17)$$

where

$$j_L(x) = \left[\frac{L^2}{4} + \frac{i\hbar}{m\omega} \left(\sin \frac{\omega x}{2} \sin \frac{\omega(t-x)}{2} \bigg/ \frac{\sin \omega t}{2} \right) \right] \tag{2.2.18}$$

To obtain the approximated density of states, equations (2.2.17) and (2.2.13) are substituted into (2.2.8). For energies deep in the tail only the ground state in the potential fluctuations should be taken into account. This corresponds to the limit $t \longrightarrow \infty$. Then the density of states becomes

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

$$\tag{2.2.19}$$

By using the formula

$$\int_{-\infty}^{\infty} dt (it)^P \exp(-\beta^2 t^2 - iqt) = 2^{-P/2} \sqrt{\pi}\beta^{-P-1} \exp(-q^2/8\beta^2) D_p(q/\beta\sqrt{2}) \tag{2.2.20}$$

One obtains

$$\rho_1(E) = \frac{1}{4}(\sqrt{2}/\pi)^{1/2} \omega^3 (m/2\pi\hbar)^{3/2} \beta^{-5/2} \exp(-q^2/8\beta^2) D_{3/2}(q/\beta\sqrt{2}) \tag{2.2.21}$$

where $q = (\frac{3}{4} E_\omega + E_o - E)/\hbar$, $E_\omega = \hbar\omega$ and $D_p(z)$ denotes the parabolic - cylinder function[34]

and

$$\beta^2 = (1/2\hbar^2)\ \xi_L(1 + 4E_L/E_\omega)^{-3/2} \tag{2.2.22}$$

$$E_L = \hbar^2/2mL^2$$

Using the asymptotic properties of the parabolic - cylinder function, $D_p(z) \underset{z\to\infty}{\simeq} \exp(-\frac{1}{4}z^2)z^P$, the density of states deep in the tail

$(E \longrightarrow -\infty$ or keeping E constant and let $\xi_L \longrightarrow 0)$ in the form proposed by Halperin and Lax is obtained.

$$\rho_1(E) = \left[(E_L/L)^3/\xi_L^2 \right] a(\nu, x) \exp\left[-E_L^2 b(\nu, x)/2\xi_L \right] \tag{2.2.23}$$

where $a(\nu, x) = (\frac{3}{4}x + \nu)^{3/2}(4 + x)^3/8\sqrt{2}\pi^2$ \tag{2.2.24}

and

$$b(\nu, x) = (\frac{3}{4}x + \nu)^2(1 + 4/x)^{3/2} \tag{2.2.25}$$

with $x = E_\omega/E_L$ and $\nu = (E_o - E)/E_L$.

The parameter ω , is introduced in the trial action S_o , will be determined from the procedure of maximizing $\rho_1(E)$, which there are three procedures, the Lloyd and Best variational principle[35], the maximizing $\rho_1(E)$ as a whole[36,37], and the minimizing the exponent $b(\nu, x)$ [36,37] as the spirit of Halperin and Lax. Here will be mention only the last case. As shown by Halperin and Lax, the maximization of the density of states deep in the tail is achieved with the sufficient accuracy when the exponential is maximum. From the condition $db(\nu, x)/dx = 0$, the best choice of x is found to be satisfied the equation :

$$x^2 + x - 4\nu = 0 \tag{2.2.26}$$

Here only the positive root is kept , because x is the ratio of the energy associated with the harmonic oscillator and the energy of the fluctuation.

$$x = \frac{1}{2} \left[(1 + 16\nu)^{1/2} - 1 \right] \tag{2.2.27}$$

The value of x that is obtained for each value of ν will be substituted into (2.2.23) and the value of $\rho_1(E)$ for each ν can be obtained.

The functions $a(\nu, x)$, $b(\nu, x)$, $n(\nu, x)$ and the kinetic energy of localization, $T(\nu, x)$ in the terms of the variable ν

only can be expressed as follows

$$a(\nu) = \left[(1 + 16\nu)^{1/2} - 1 \right]^{3/2} \left[(1 + 16\nu)^{1/2} + 7 \right]^{9/2} /2^{12}\sqrt{2}\ \pi^2 \quad (2.2.28)$$

$$b(\nu) = \left[(1 + 16\nu)^{1/2} - 1 \right]^{1/2} \left[(1 + 16\nu)^{1/2} + 7 \right]^{7/2} /2^8 \quad (2.2.29)$$

$$n(\nu) = 32\nu/ \left[(1 + 16\nu)^{1/2} - 1 \right]\left[(1 + 16\nu)^{1/2} + 7 \right] \quad (2.2.30)$$

and

$$T(\nu) = \frac{3}{8}\left[(1 + 16\nu)^{1/2} - 1 \right] \quad (2.2.31)$$

Sa-yakanit considers the limiting values of $a(\nu, x)$ and $b(\nu, x)$ in two cases, when $\nu \ll 1$ and $\nu \gg 1$ respectively.
For $\nu \ll 1$,

$$a(\nu) = 32\sqrt{2}\nu^{3/2}/\pi^2 \quad (2.2.32)$$

and

$$b(\nu) = 16\nu^{1/2} \quad (2.2.33)$$

For $\nu \gg 1$,

$$a(\nu) = \nu^3/\sqrt{2}\pi^2 \quad (2.2.34)$$

and

$$b(\nu) \quad = \quad \nu^2 \qquad\qquad (2.2.35)$$

2.2.3 Screened Coulomb Potential

For an impurity of the screened Coulomb form

$$\eta v(\vec{x}(\tau) - \vec{R}) \quad = \quad \frac{-Z e^2 \exp}{\varepsilon_o |\vec{x}(\tau)-\vec{R}|} (-Q |\vec{x}(\tau) - \vec{R}|) \qquad (2.2.36)$$

the autocorrelation function can be written

$$W(\vec{x}(\tau)-\vec{x}(\sigma)) \quad = \quad (2\pi e^4 Z^2/Q\varepsilon_o^2)\exp\left[-Q|\vec{x}(\tau)-\vec{x}(\sigma)| \right] \qquad (2.2.37)$$

The action associated with the above autocorrelation function is

$$S \quad = \quad \int_o^t d\tau \, \frac{m}{2} \dot{\vec{x}}^2(\tau) - \int_o^t d\tau \, E_o + \frac{i}{2\hbar} \xi_Q \int_o^t \int_o^t d\tau d\sigma \exp\left[-Q|\vec{x}(\tau)-\vec{x}(\sigma)| \right],$$

$$(2.2.38)$$

where $\xi_Q = 2\pi Z^2 e^4 N/Q\varepsilon_o^2$ has the dimension of the energy square.

After writing $W(\vec{x}(\tau) - \vec{x}(\sigma))$ in terms of Fourier components the average $\langle S - S_o \rangle_{S_o}$ becomes

$$\langle S-S_o \rangle_{S_o} = -E_o t + \frac{i}{2\hbar} \xi_Q \frac{\Omega t}{2\pi} \int_0^t dx \int \frac{d\vec{k}}{(2\pi)^3} \left(\frac{4\pi}{\vec{K}^2 + \Omega^2}\right)^2 \exp\left[-\frac{k^2}{2}\frac{i\hbar}{m\omega}\right.$$

$$\left. \times (\sin\frac{\omega x}{2} \sin\frac{\omega(t-x)}{2}/\sin\frac{\omega t}{2})\right] - \frac{3}{2} i\hbar(\frac{\omega t}{2}\cot\frac{\omega t}{2} - 1).$$

$$(2.2.39)$$

Inserting the identity

$$(\vec{K}^2 + Q^2)^{-2} = \int_0^\infty dy\, y \exp\left[-(\vec{K}^2 + Q^2)y\right]$$

$$(2.2.40)$$

into (2.2.39) and performing the $\vec{K}$ integration, one gets

$$\langle S-S_o \rangle_{S_o} = -E_o t + \frac{i}{2\hbar} \xi_Q \frac{\Omega t}{\sqrt{\pi}} \int_0^t dx \int_0^\infty dy\, y \exp(-Q^2 y) \left[j_y(x)\right]^{-3/2}$$

$$- \frac{3}{2} i\hbar(\frac{\omega t}{2}\cot\frac{\omega t}{2} - 1)$$

$$(2.2.41)$$

where

$$j_y(x) = \left[y + \frac{i\hbar}{m\omega}(\sin\frac{\omega x}{2} \sin\frac{\omega(t-x)}{2}/\sin\frac{\omega t}{2})\right]$$

$$(2.2.42)$$

The approximate density of states is obtained by substituting (2.2.39) and (2.2.11) into (2.2.6). For energies deep in the tail,

the ground state contribution is considered at $t \longrightarrow \infty$

then the density of states becomes

$$\rho_1(E) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \; (\frac{m}{2\pi i\hbar t})^{3/2} (i\omega t)^3$$

$$\times \exp\left[-\frac{3}{4} i\omega t - \frac{i}{\hbar} (E_o - E)t - \frac{\xi_Q Q t^2}{2\hbar^2\sqrt{\pi}} \int_{o}^{\infty} dy \; y \; \exp(-Q^2 y)(y+\hbar/2m\omega)^{-3/2} \right],$$

$$(2.2.43)$$

After integrating (2.2.43) by using the formula (2.2.18), the density

of states in tail region can be expressed in terms of two dimensionless

functions, $a(\nu, z)$ and $b(\nu, z)$ as follow

$$\rho_1(E) = \frac{Q^3}{E_Q \xi^{5/4}} \frac{a(\nu,z)}{(b(\nu,z))^{3/4}} \exp\left[-b(\nu,z)/4\xi' \right] D_{3/2}\left[(b(\nu, z)/\xi')^{1/2} \right],$$

$$(2.2.44)$$

In the limit of large $b(\nu, z)/\xi'$ $(\xi \longrightarrow o)$ the asymptotic expression

for the parabolic cylinder function is

$$D_p(x) = \exp(-x^2/4) x^P\left[1 - P(\frac{P-1}{2}) \frac{1}{x^2} + \ldots \right] \qquad (2.2.45)$$

If only the first term of (2.2.45) is kept then the density of states

in (2.2.44) becomes

$$\rho_1(E) = \left[(E_Q Q)^3/\xi_Q^2 \right] a(\nu,z) \exp\left[-E_Q^2 b(\nu,z)/2\xi_Q \right] \qquad (2.2.46)$$

where

$$a(\nu,z) = (\tfrac{3}{2}z^{-2} + \nu)^{3/2}/8\pi\sqrt{2}\ z^6 \exp(\tfrac{1}{2}z^2)\ D_{-3}^2(z) \qquad (2.2.47)$$

and

$$b(\nu, z) = \sqrt{\pi}\quad (\tfrac{3}{2}z^{-2} + \nu)^2/\ 2\sqrt{2}\ \exp(\tfrac{1}{4}z^2)\ D_{-3}(z) \qquad (2.2.48)$$

with $z = (2E_Q/E_\omega)^{1/2}$ and $\xi' = \xi_Q/E_Q^2$.

Similarly to the Gaussian potential case, the maximization of the density of states deep in the tail is achieved with a sufficient accuracy when the exponential is maximium. From the condition $db(\nu, z)/dz = 0$, one obtains the following equation for the best choice of parameter z,

$$D_{-3}(z) = \tfrac{1}{2} z^3 (\tfrac{3}{2} z^{-2} + \nu)\ D_{-4}(z) \qquad (2.2.49)$$

The value of z that is obtained for each value of ν is substituted back into (2.2.46). The value of $\rho_1(E)$ for each ν can be obtained.

The other two quantities of interest are $n(\nu, z)$ and $T(\nu, z)$ can be expressed as follows

$$n(\nu, z) \quad = \quad 2\nu/(\frac{3}{2} z^2 - \nu) \tag{2.2.50}$$

and

$$T(\nu, z) \quad = \quad \frac{3}{2} z^{-2} \tag{2.2.51}$$

Sa-yakanit considers the limiting values of $a(\nu, z)$, $b(\nu, z)$ $n(\nu, z)$ and $T(\nu, z)$ in two limiting cases, strong screening and weak screening respectively.

For strong screening $(Q \longrightarrow \infty)$ which is equivalent to $\nu \ll 1$ or $z \longrightarrow \infty$, the limiting value of z obtained by substituting the asymptotic form of parabolic cylinder function $D_p(z) \underset{z \to \infty}{\simeq} \exp(-\frac{1}{4}z^2) z^P$ into (2.2.49) is

$$z \quad = \quad (2\nu)^{-1/2} \tag{2.2.52}$$

and consequently, one obtains

$$a(\nu, z) \quad = \quad \nu^{3/2}/\sqrt{2}\pi \tag{2.2.53}$$

$$b(\nu, z) \quad = \quad 2\sqrt{\pi} \; \nu^{1/2} \tag{2.2.54}$$

$$n(\nu, z) \quad = \quad \frac{1}{2} \tag{2.2.55}$$

and $\quad T(\nu, z)/\nu \quad = \quad 3 \tag{2.2.56}$

For weak screening $(Q \longrightarrow 0)$, or equivalently, $\nu \gg 1 (z \longrightarrow 0)$, substituting the asymptotic forms of the parabolic - cylinder functions $D_{-3}(z) \underset{z \longrightarrow 0}{\simeq} \frac{1}{2} \sqrt{\frac{\pi}{2}}$ and $D_{-4}(z) \underset{z \to 0}{\simeq} \frac{1}{3}$ into (2.2.49) and using the assumption $z^{-2} \ll \nu$, the limiting value of z obtained is

$$z = \left[3(\pi/2)^{1/2} \right]^{1/3} \nu^{-1/3} \qquad (2.2.57)$$

and consequently one obtains

$$a(\nu, z) \simeq \sqrt{2}/(9\pi^3) \; \nu^{7/2} \qquad (2.2.58)$$

$$b(\nu, z) \simeq \nu^2 \qquad (2.2.59)$$

$$n(\nu, z) = 2 \qquad (2.2.60)$$

and

$$T(\nu, z)/\nu = 0 \qquad (2.2.61)$$