CHAPTER III

THE SIMPLIFIED APPROACH OF THE HALPERIN AND LAX THEORY

It is not too much of an exaggeration to say that Halperin and Lax theory[25,26] is the most complete theory of the deep tail state in heavily doped semiconductors. However, their theory is the complicate one ; their results are obtained by a very complicate calculation using large computer program. For this reason, in this chapter, the simplified approach of the Halperin and Lax theory is presented. The solving of Hartree-Fock like equation is used in this work. This means that the numerically solving for the wave functions (which was done by Halperin and Lax) is represented by using the appropriate wave functions. Then the variational principle is used for adjusting the parameters in the wave function, in order to maximize the density of states for each energy.

3.1 Screened Coulomb Potential

For an impurity potential having the screened Coulomb form

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

there are two methods to be introduced ; Eymard and Duraffourg method and present method.

3.1.1 Eymard and Duraffourg Method

Eymard and Duraffourg[31] assumed that the initial wave function satisfying the Hartree-Fock equation is the Hydrogen-like wave function,

$$\phi(r) = (\alpha^3/\pi)^{1/2} \exp(-\alpha r) \tag{3.1.1}$$

Then

$$S(r) = (4\alpha^3)^{1/2} r \exp(-\alpha r) \tag{3.1.2}$$

where α is the variational parameter. Since $U(r) = \int K(r,r') S^2(r') dr'$, thus

$$U(r) = 4\alpha^3 \int_0^\infty K(r,r') r'^2 \exp(-2\alpha r') dr' \tag{3.1.3}$$

Here $K(r,r')$ is expressed in the units where $Q = \hbar^2/2m = 1$

$$K(r,r') = (rr')^{-1} e^{-r_>} \left[(r_> + 1)\sinh r_< - r_< \cos hr_<\right] \tag{3.1.4}$$

Hence

$$U(r) = (4\alpha^3/r) \int_0^\infty r' \left[(r_> + 1)\sin hr_< - r_< \cos hr_<\right] \exp\left[-(2\alpha r' + r_>)\right] dr' \tag{3.1.5}$$

To evaluate the integral of equation (3.1.5), the limit of the integral must be separated into $o \rightarrow r$ and $r \rightarrow \infty$.

$$U(r) = (4\alpha^3/r)\left[e^{-r}\int_0^r r'\left[(r+1)\sin hr' - r'\cos hr' \right] \exp(-2\alpha r')dr' \right.$$

$$\left. + \int_r^\infty r'\left[(r'+1)\sin hr - r\cos hr \right] \exp\left[-(2\alpha+1)r' \right] dr' \right] \quad (3.1.6)$$

As a preliminary of determining the function $U(r)$ in (3.1.6) let

$$U(r) = (4\alpha^3/r)\left[U_1(r) + U_2(r) \right] \quad (3.1.7)$$

where $$U_1(r) = e^{-r}\int_0^r r'\left[(r+1)\sin hr' - r'\cos hr' \right] \exp(-2\alpha r')dr' \quad (3.1.8)$$

and

$$U_2(r) = \int_r^\infty r'\left[(r'+1)\sin hr - r\cos hr \right] \exp\left[-(2\alpha+1)r' \right] dr' \quad (3.1.9)$$

By using the definition of $\sin hx = (e^x - e^{-x})/2$, $\cos hx = (e^x + e^{-x})/2$

and the formula $\int_0^U x^n e^{-ax}dx = \frac{n!}{a^{n+1}} - e^{-Ua} \sum_{K=o} \frac{n!}{K!} \frac{U^k}{a^{n-k+1}} \left[U > o,\ \mathrm{Re}\,a > o \right]$.

One gets

$$U_1(r) = \left[2^{1/3}(4\alpha^2-1) \right]^{-3} \left[\left[(32\alpha^3-8\alpha)r - 32\alpha \right] e^{-r} + (2\alpha+1)^3\left[3-2\alpha-(4\alpha^2-6\alpha+2)r \right] e^{-2\alpha r} \right.$$

$$\left. + (2\alpha-1)^3\left[(2\alpha+3)+(4\alpha^2+10\alpha+4)r + (8\alpha^2+8\alpha+2)r^2 \right] e^{-(2\alpha+2)r} \right] \quad (3.1.10)$$

Similarly, using the formula

$$\int_{U}^{\infty} x^{n}\, e^{-ax} dx = e^{-aU} \sum_{K=o}^{n} \frac{n!}{K!} \frac{U^{k}}{a^{(n-k+1)}} \quad [\, U > 0,\ \mathrm{Re}\, a > 0\,]$$

one has

$$U_2(r) = [\, 2^{1/3}(2\alpha+1)\,]^{-3} \Big[[(2\alpha+3) + (4\alpha^2 + 6\alpha + 2)r]\, e^{-2\alpha r}$$

$$- [\, (2\alpha+3) + (4\alpha^2+10\alpha+4)r + (8\alpha^2+ 8\alpha+2)r^2\,]\, e^{-(2\alpha+2)r} \Big]$$

(3.1.11)

Combining the results for $U_1(r)$ and $U_2(r)$ and re-arranging, one obtains

$$U(r) = 8\alpha^3 \left[\frac{[(8\alpha^3-2\alpha)r-8\alpha]e^{-r} + [\, 8+(4\alpha^2-1)r\,]\, e^{-2\alpha r}}{r(4\alpha^2-1)^3} \right] \quad (3.1.12)$$

Consider Hartree-Fock like equation

$$[\, d^2/dr^2 + \mu U(r)\,]\, S(r) = \nu S(r) \quad (3.1.13)$$

Multiply each side of this equation by $S(r)$ and integrate throughout the configuration space of the system with using the normalization condition of $S(r)$.

$$\int_0^\infty S(r)^2\, dr = 4\alpha^3 \int_0^\infty r^2 e^{-2\alpha r}\, dr = 1$$

one has

$$\int_0^\infty S(r) \frac{d^2}{dr^2} [\, S(r)\,] dr + \mu \int_0^\infty U(r) [\, S(r)\,]^2\, dr = \nu \qquad (3.1.14)$$

Let $$\theta_o = \int_0^\infty S(r) \frac{d^2}{dr^2} [\, S(r)\,] dr \qquad (3.1.15)$$

and

$$\sigma_o^2 = \int_0^\infty U(r) [S(r)]^2\, dr \qquad (3.1.16)$$

Now equation (3.1.14) may be written in the form

$$\theta_o + \mu\sigma_o^2 = \nu \qquad (3.1.17)$$

Differentiating $S(r)$ in (3.1.2) with respect to r twice and substituting into (3.1.15) , one finds

$$\theta_o = 4\alpha^5 \int_0^\infty r^2 e^{-2\alpha r}\, dr - 8\alpha^4 \int_0^\infty r e^{-2\alpha r}\, dr \qquad (3.1.18)$$

Applying formula

$$\int_0^\infty x^n e^{-ax} dx = n!/a^{(n+1)}, [n > -1, \quad a > 0] \tag{3.1.19}$$

equation (3.1.18) becomes

$$\theta_o = -\alpha^2 \tag{3.1.20}$$

Substituting U(r) and S(r) into (3.1.16) gives

$$\sigma_o^2 = [32\alpha^6/(4\alpha^2 - 1)^3][(8\alpha^3 - 2\alpha) \int_0^\infty r^2 e^{-(2\alpha+1)r} dr$$

$$-8\alpha \int_0^\infty r e^{-4\alpha r} dr + (4\alpha^2 - 1) \int_0^\infty r^2 e^{-4\alpha r} dr] \tag{3.1.21}$$

Using the formula in (3.1.19) the simple form of σ_o^2 is obtained

$$\sigma_o^2 = [\alpha^3(32\alpha^2 + 10\alpha + 1)/(2\alpha + 1)^5] \tag{3.1.22}$$

Substituting the values of θ_o and σ_o^2 into equation (3.1.17) one obtains

$$\mu = [(\nu + \alpha^2)(2\alpha + 1)^5/\alpha^3(32\alpha^2 + 10\alpha + 1)] \tag{3.1.23}$$

σ_1^2 can be calculated by using equation (2.1.65)

$$(\sigma_1^2 = -\frac{1}{3}\int_0^\infty r\,U(r)dr\,[\,S^2(r)/r\,]''\,)$$

Thus, $\sigma_1^2 = [\,4\alpha^5(10\alpha + 1)/3(2\alpha + 1)^5\,]$ (3.1.24)

The two dimensionless functions $a(\nu)$ and $b(\nu)$ are obtained by substituting the values of σ_o , σ_1 and μ into the appropriate equations

$$a(\nu) = \frac{2(1 + 10x)^{3/2}(1 + 2x)^{10}(\nu + x^2)^3}{3\sqrt{3}\,\pi^2 x^3(1 + 10x + 32x^2)^{7/2}} \qquad (3.1.25)$$

and

$$b(\nu) = \frac{(\nu + x^2)^2(2x + 1)^5}{x^3(1 + 10x + 32x^2)} \qquad (3.1.26)$$

with $x = \alpha/Q$.

From (2.1.62) the density of states in the notation of Halperin and Lax is

$$\rho(E) = [\,(E_Q Q)^3/\xi^2\,]\; a(\nu)\, \exp[\,-E_Q^2\, b(\nu)/2\xi\,] \qquad (3.1.27)$$

It is clear that when $\xi \rightarrow 0$, the exponential factor will become very sensitive to the choice of x while the other factors are much more slowly varying. Hence the best choice of x is that which minimizes $b(\nu)$, i.e. differentiating (3.1.26) with respect to x and setting it equal to zero. One has

$$\frac{\nu}{x^2} = \frac{(1 + 12x + 68x^2 + 256x^3)}{(3 + 36x + 140x^2)} \tag{3.1.28}$$

The complete determination of (3.1.25), (3.1.26), and (3.1.27) requires the solution of (3.1.28).

Beside the two dimensionless functions $a(\nu)$ and $b(\nu)$ other quantities of interest are $n(\nu)$ and $T(\nu)$, where $n(\nu)$ is defined by

$$n(\nu) = \frac{d \log b(\nu)}{d \log \nu} = \frac{2\nu}{(\nu+x^2)} \tag{3.1.29}$$

and the kinetic energy of localization is

$$T(\nu) = \mu\sigma_o^2 - \nu = x^2 \tag{3.1.30}$$

Now consider the limiting values of these functions. For strong screening $\nu << 1$ or equivalently , $Q \longrightarrow \infty$ (or $x = \frac{\alpha}{Q} \longrightarrow 0$) equation (3.1.28) yields

$$x \simeq (3\nu)^{1/2} \tag{3.1.31}$$

If the higher order terms of x are neglected, (3.1.25), (3.1.26), (3.1.29), and (3.1.30) will become :

$$a(\nu) = [\ 2(\nu + x^2)^3/3\sqrt{3}\ \ \pi^2 x^3\ ] = 0.48\nu^{3/2} \tag{3.1.32}$$

$$b(\nu) \simeq [(\nu + x^2)^2/x^3] = 3.07\nu^{1/2} \tag{3.1.33}$$

$$n(\nu) \simeq [2\nu/(\nu + 3\nu)] = \frac{1}{2} \tag{3.1.34}$$

$$T(\nu) \simeq 3\nu \tag{3.1.35}$$

Similarly, for weak screening $\nu >> 1$ ($Q \longrightarrow 0$ or $x \longrightarrow \infty$), keeping only the higher order terms of x equation (3.1.28) has a solution

$$x \simeq 0.82\nu^{1/3} \tag{3.1.36}$$

and consequently one obtains

$$a(\nu) \simeq \frac{2(10x)^{3/2}(2x)^{10}\nu^3}{3\sqrt{3}\,\pi^2 x^3 (32x^2)^{7/2}} = 5.06 \times 10^{-3}\nu^{7/2} \tag{3.1.37}$$

$$b(\nu) \simeq [\nu^2(2x)^5/32x^5] = \nu^2 \tag{3.1.38}$$

$$n(\nu) \simeq 2\nu/\nu = 2 \tag{3.1.39}$$

and

$$T(\nu)/\nu \simeq (0.82)^{2/3}\nu^{-1/3} \longrightarrow 0 \tag{3.1.40}$$

The numerical values of x, $n(\nu)$, and $T(\nu)$, for each value of the energy ν are shown in Table 3.1 , $a(\nu)$ and $b(\nu)$ are shown in Table 3.2, σ_o^2, σ_1^2, and μ are shown in Table 3.3.

Table 3.1 Numerical results of the kinetic energy of localization, $T(\nu)$, the logarithmic derivative of the exponent $b(\nu)$, $n(\nu)$, and of the adjustable parameter, x.

ν	x	$T(\nu)$	$n(\nu)$
$1x10^{3}$	8.1739	6.6813x10	1.8747
$6x10^{2}$	6.8934	4.7519x10	1.8532
$2x10^{2}$	4.7779	2.2828x10	1.7951
$1x10^{2}$	3.7909	1.4371x10	1.7487
6x10	3.1963	1.0216x10	1.7090
2x10	2.2136	4.9000	1.6064
1x10	1.7548	3.0795	1.5291
6	1.4783	2.1853	1.4660
2	1.0207	1.0418	1.3150
1	$8.0657x10^{-1}$	$6.5056x10^{-1}$	1.2117
$6x10^{-1}$	$6.7721x10^{-1}$	$4.5861x10^{-1}$	1.1336
$2x10^{-1}$	$4.6233x10^{-1}$	$2.1375x10^{-1}$	$9.6678x10^{-1}$
$1x10^{-1}$	$3.6118x10^{-1}$	$1.3045x10^{-1}$	$8.6786x10^{-1}$
$6x10^{-2}$	$2.9980x10^{-1}$	$8.9879x10^{-2}$	$8.0064x10^{-1}$
$2x10^{-2}$	$1.9739x10^{-1}$	$3.8965x10^{-2}$	$6.7837x10^{-1}$
$1x10^{-2}$	$1.4927x10^{-1}$	$2.2283x10^{-2}$	$6.1953x10^{-1}$
$6x10^{-3}$	$1.2038x10^{-1}$	$1.4491x10^{-2}$	$5.8562x10^{-1}$
$2x10^{-3}$	$7.3777x10^{-2}$	$5.4430x10^{-3}$	$5.3742x10^{-1}$
$1x10^{-3}$	$5.3298x10^{-2}$	$2.8407x10^{-3}$	$5.2074x10^{-1}$

Table 3.2 Numerical results of the dimensionless functions, $a(\nu)$, $b(\nu)$ and of the adjustable parameter, x.

ν	x	$a(\nu)$	$b(\nu)$
1×10^{3}	8.1739	3.1209×10^{8}	1.4744×10^{6}
6×10^{2}	6.8934	5.8867×10^{7}	5.6889×10^{5}
2×10^{2}	4.7779	1.7522×10^{6}	7.6558×10^{4}
1×10^{2}	3.7909	2.0321×10^{5}	2.2407×10^{4}
6×10	3.1963	4.3137×10^{4}	9.2631×10^{3}
2×10	2.2136	1.7523×10^{3}	1.4958×10^{3}
1×10	1.7548	2.5834×10^{2}	5.0428×10^{2}
6	1.4783	6.6939×10	2.3461×10^{2}
2	1.0207	4.4453	5.0832×10
1	8.0657×10^{-1}	9.2839×10^{-1}	2.1169×10
6×10^{-1}	6.7721×10^{-1}	3.1524×10^{-1}	1.1629×10
2×10^{-1}	4.6233×10^{-1}	3.8038×10^{-2}	3.6708
1×10^{-1}	3.6118×10^{-1}	1.1464×10^{-2}	1.9445
6×10^{-2}	2.9980×10^{-1}	5.0164×10^{-3}	1.2701
2×10^{-2}	1.9739×10^{-1}	9.6165×10^{-4}	5.6536×10^{-1}
1×10^{-2}	1.4927×10^{-1}	3.5878×10^{-4}	3.6086×10^{-1}
6×10^{-3}	1.2038×10^{-1}	1.7553×10^{-4}	2.6534×10^{-1}
2×10^{-3}	7.3777×10^{-2}	3.7591×10^{-5}	1.4359×10^{-1}
1×10^{-3}	5.3298×10^{-2}	1.3977×10^{-5}	9.9557×10^{-2}

Table 3.3 Numerical results of the functions σ_o^2, σ_1^2 and μ for each values of the energy ν.

ν	σ_o^2	σ_1^2	μ
$1x10^{3}$	$7.7190x10^{-1}$	2.5619	$1.3820x10^{3}$
$6x10^{2}$	$7.3701x10^{-1}$	2.0531	$8.7857x10^{2}$
$2x10^{2}$	$6.4856x10^{-1}$	1.2357	$3.4357x10^{2}$
$1x10^{2}$	$5.8377x10^{-1}$	$8.7259x10^{-1}$	$1.9592x10^{2}$
6x10	$5.3225x10^{-1}$	$6.6406x10^{-1}$	$1.3192x10^{2}$
2x10	$4.1451x10^{-1}$	$3.482x10^{-1}$	6.0070x10
1x10	$3.3924x10^{-1}$	$2.2065x10^{-1}$	3.8555x10
6	$2.8558x10^{-1}$	$1.5322x10^{-1}$	2.8662x10
2	$1.8202x10^{-1}$	$6.3610x10^{-2}$	1.6711x10
1	$1.2869x10^{-1}$	$3.3864x10^{-2}$	1.2826x10
$6x10^{-1}$	$9.6366x10^{-2}$	$2.0402x10^{-2}$	1.0985x10
$2x10^{-1}$	$4.6635x10^{-2}$	$5.9966x10^{-2}$	8.8720
$1x10^{-1}$	$2.7312x10^{-2}$	$2.4935x10^{-3}$	8.4376
$6x10^{-2}$	$1.7687x10^{-2}$	$1.1233x10^{-3}$	8.4739
$2x10^{-2}$	$6.1498x10^{-3}$	$2.2512x10^{-4}$	9.5881
$1x10^{-2}$	$2.8879x10^{-3}$	$6.6718x10^{-5}$	1.1178x10
$6x10^{-3}$	$1.5824x10^{-3}$	$2.5259x10^{-5}$	1.2949x10
$2x10^{-3}$	$3.8581x10^{-4}$	$2.5449x10^{-6}$	1.9292x10
$1x10^{-3}$	$1.4817x10^{-4}$	$5.2979x10^{-7}$	2.5922x10

Table 3.4 Numerical results of the density of states in units of $(\Omega^3/E_\Omega \xi'^2)$ for $\xi' = \xi/E_\Omega^2 = 0.05, 0.5, 5$ and 50 respectively.

ν	$\rho(\varepsilon)$			
	$\xi' = 50$	$\xi'=5$	$\xi'=0.5$	$\xi'=0.05$
1×10^{3}	0.0	0.0	0.0	0.0
6×10^{2}	0.0	0.0	0.0	0.0
2×10^{2}	0.0	0.0	0.0	0.0
1×10^{2}	0.0	0.0	0.0	0.0
6×10	2.5458×10^{-36}	0.0	0.0	0.0
2×10	5.5928×10^{-4}	1.9217×10^{-62}	0.0	0.0
1×10	1.6677	3.2479×10^{-20}	0.0	0.0
6	6.4089	4.3228×10^{-9}	0.0	0.0
2	2.6739	2.7561×10^{-2}	3.7305×10^{-22}	0.0
1	7.5126×10^{-1}	1.1177×10^{-1}	5.9404×10^{-10}	0.0
6×10^{-1}	2.8063×10^{-1}	9.8533×10^{-2}	2.8062×10^{-6}	9.8495×10^{-52}
2×10^{-1}	3.6667×10^{-2}	2.6351×10^{-2}	9.6833×10^{-4}	4.3482×10^{-18}
1×10^{-1}	1.1244×10^{-2}	9.4385×10^{-3}	1.6401×10^{-3}	4.1171×10^{-11}
6×10^{-2}	4.9531×10^{-3}	4.4181×10^{-3}	1.4087×10^{-3}	1.5294×10^{-8}
2×10^{-2}	9.5623×10^{-4}	9.0879×10^{-4}	5.4637×10^{-4}	3.3705×10^{-6}
1×10^{-2}	3.5749×10^{-4}	3.4606×10^{-4}	2.5009×10^{-4}	9.7189×10^{-6}
6×10^{-3}	1.7306×10^{-4}	1.7093×10^{-4}	1.3462×10^{-4}	1.2359×10^{-5}
2×10^{-3}	3.7538×10^{-5}	3.7056×10^{-5}	3.2563×10^{-5}	8.9429×10^{-6}
1×10^{-3}	1.3963×10^{-5}	1.3838×10^{-5}	1.2652×10^{-5}	5.1645×10^{-6}

The density of states for each value of ξ' are shown in Table 3.4. These results are obtained by using computer program given in Appendix A.

3.1.2 Present Method

The trial wave function is assumed to be in the form

$$\phi(r) = [(2\beta^4)/3\pi]^{1/2}\, r^{1/2} \exp(-\beta r) \qquad (3.1.41)$$

Since $S(r) = (4\pi)^{1/2}\, r\phi(r)$ then

$$S(r) = [(8\beta^4)/3]^{1/2}\, r^{3/2} \exp(-\beta r) \qquad (3.1.42)$$

where β is an adjustable parameter, and $S(r)$ is a normalized function.

$$\int_0^\infty [S(r)]^2\, dr = [(8\beta^4/3)] \int_0^\infty r^3\, e^{-2\beta r}\, dr = 1 \qquad (3.1.43)$$

A shape of $S(r)$ in (3.1.42) is more similar to the numerically $S(r)$ (in Halperin and Lax theory) than $S(r)$ in Eymard and Duraffourg method. (see Fig. 3.1).

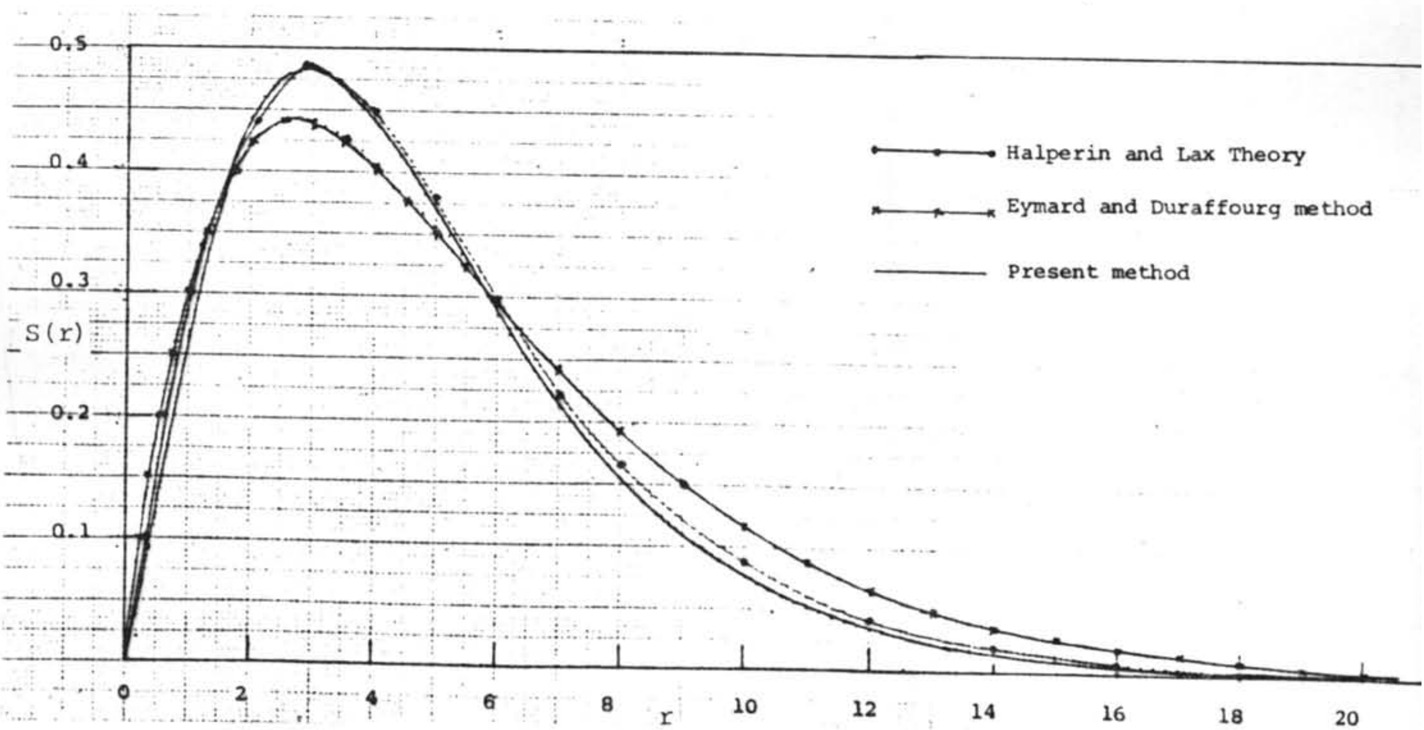

Fig. 3.1 The wave function $S(r)$, plotted against r in dimensionless units for $\nu = 0.1$.

To determine the density of states, it is needed to know the two dimensionless functions $a(\nu)$ and $b(\nu)$. Since these functions are expressed in terms of functions σ_o, σ_1, and μ. Therefore the function $U(r)$ must be known,

$$U(r) = (8\beta^4/3r) \int_0^\infty [(r_> + 1)\sinh r_< - r_< \cosh r_<]\, r'^2 \exp[-(2\beta r' + r_>)]\, dr', \tag{3.1.44}$$

$$= [16\beta^4/3r(4\beta^2-1)^4] \Big[[(48\beta^4 - 8\beta^2 - 1)r - (80\beta^2+4)] e^{-r} + [(80\beta^2+4) + (64\beta^3 - 16\beta)r + (16\beta^4 - 8\beta^2 + 1)r^2]\, e^{-2\beta r} \Big] \tag{3.1.45}$$

Then the θ_0 is obtained from equation (3.1.15),

$$\theta_o = (8\beta^4/3)\left[(3/4) \int_0^\infty r\, e^{-2\beta r}\, dr - 3\beta \int_0^\infty r^2 e^{-2\beta r} dr + \beta^2 \int_0^\infty r^3 e^{-2\beta r}\, dr\right]$$

$$= -\beta^2/2 \qquad (3.1.46)$$

Substituting the values of U(r) and S(r) in equation (3.1.16) one gets

$$\sigma_o^2 = [128\beta^8/9(4\beta^2-1)^4]\Big[(48\beta^4-8\beta^2-1)\int_0^\infty r^3 e^{-(2\beta+1)r}\, dr - (80\beta^2+4)\int_0^\infty r^2 e^{-(2\beta+1)r} dr$$

$$+ (80\beta^2+4)\int_0^\infty r^2 e^{-4\beta r}\, dr + (64\beta^4-16\beta)\int_0^\infty r^3 e^{-4\beta r}\, dr$$

$$+ (16\beta^4-8\beta^2+1)\int_0^\infty r^4 e^{-4\beta r}\, dr\Big]$$

$$= [\beta^3(1152\beta^4+728\beta^3+244\beta^2+42\beta+3)/9(2\beta+1)^7] \qquad (3.1.47)$$

Then combining the results of θ_o and σ_o^2, one finds

$$\mu = \frac{9(2\nu+\beta^2)(2\beta+1)^7}{2\beta^3(1152\beta^4+728\beta^3+244\beta^2+42\beta+3)} \qquad (3.1.48)$$

To calculate σ_1^2 the following equation is used.

$$\sigma_1^2 = -\frac{1}{3}\int_0^\infty r\,U(r)\,dr\,[\,S(r)^2/r\,]'' \tag{3.1.49}$$

where $[\,S(r)^2/r\,]''$ denotes the second derivative of $S(r)^2/r$ which equal to

$$[S(r)^2/r\,]'' = (16/3)\beta^4\,(1 - 4\beta r + 2\beta^2 r^2)e^{-2\beta r} \tag{3.1.50}$$

Substituting the above equation into (3.1.49) , yields

$$\sigma_1^2 = (-16\beta^4/9)(\sigma_{1a}^2 - \sigma_{1b}^2 + \sigma_{1c}^2) \tag{3.1.51}$$

where

$$\sigma_{1a}^2 = \int_0^\infty r\,U(r)\,\exp\,(-2\beta r)dr$$

$$= \frac{16\beta^4}{3(4\beta^2-1)^4}\left[\frac{(96\beta^5-272\beta^4-336\beta^3-104\beta^2-18\beta-5)}{(2\beta+1)^3} + \frac{(784\beta^4-8\beta^2+1)}{32\beta^3}\right] \tag{3.1.52}$$

$$\sigma_{1b}^2 = 4\beta\int_0^\infty r^2\,U(r)\,\exp\,(-2\beta r)dr$$

$$= \frac{64\beta^5}{3(4\beta^2-1)^4}\left[\frac{(96\beta^5-160\beta^4-96\beta^3-8\beta^2-6\beta)}{(2\beta+1)^3} + \frac{(944\beta^4-56\beta^2+3)}{128\beta^3}\right] \tag{3.1.53}$$

and

$$\sigma_{1c}^2 = 2\beta^2 \int_0^\infty r^3\ U(r)\ \exp\ (-2\beta r)dr$$

$$= \frac{32\beta^6}{3(4\beta^2-1)^4}\left[\frac{(144\beta^5-232\beta^4+12\beta^3-14\beta^2)}{(2\beta+1)^3} + \frac{(560\beta^4-56\beta^2+3)}{128\beta^3}\right] \quad (3.1.54)$$

Thus

$$\sigma_1^2 = \frac{4\beta^4(264\beta^3+60\beta^2+14\beta+1)}{27(2\beta+1)^7} \quad (3.1.55)$$

Now the values of $a(\nu)$ and $b(\nu)$ can be solved.

$$a(\nu) = \frac{546(2\nu+y^2)^3(2y+1)^{14}(264y^3+60y^2+14y+1)^{3/2}}{(27)^{3/2}\pi^2 y^3(1152y^4+728y^3+244y^2+42y+3)^{7/2}} \quad (3.1.56)$$

and

$$b(\nu) = \frac{9(2\nu+y^2)^2(2y+1)^7}{4y^3(1152y^4+728y^3+244y^2+42y+3)} \quad (3.1.57)$$

where $y = \beta/Q$ is given. By using the variational principle :

$$db(\nu)/dy = 0$$

Thus :

$$\frac{2\nu}{y^2} = \frac{(9216y^5+3828y^4+1472y^3+344y^2+48y+3)}{(6604y^4+3392y^3+968y^2+144y+9)} \quad (3.1.58)$$

The logarithmic derivative $n(\nu)$ and the kinetic energy of localization $T(\nu)$ are also obtained as Eymard and Duraffourg method, i.e.

$$n(\nu) = \frac{d}{d\nu}\log b(\nu) \Big/ \frac{d}{d\nu}\log\nu = \frac{4\nu}{(2\nu+y^2)} \tag{3.1.59}$$

and

$$T(\nu) = \mu\,\sigma_o^2 - \nu = y^2/2 \tag{3.1.60}$$

An other interesting result is the analytical asymptotic expression of the density of states. For both limiting values of ν, i.e., $\nu >> 1$ and $\nu << 1$, the asymptotic expression of the functions $a(\nu)$, $b(\nu)$, $n(\nu)$, and $T(\nu)$ are shown in Table 3.5

The numerical results of y, $n(\nu)$, and $T(\nu)$ for each value of the energy ν are shown in Table 3.6, $a(\nu)$, and $b(\nu)$ are shown in Table 3.7, σ_o^2, σ_1^2 and μ are shown in Table 3.8 and the density of states for each value of ξ' are shown in Table 3.9. These results are obtained by using computer program given in Appendix B.

Table 3.5 The limiting values of $a(\nu)$, $b(\nu)$, $n(\nu)$, and $T(\nu)$

	$\nu \ll 1$ ($Q \to \infty$, or $y \to 0$)	$\nu \gg 1$ ($Q \to 0$, $y \to \infty$)
y	$(6\nu)^{1/2}$	$1.12\nu^{1/3}$
$a(\nu)$	$0.29\nu^{3/2}$	$0.42 \times 10^{-2}\ \nu^{7/2}$
$b(\nu)$	$3.2\ \nu^{1/2}$	ν^{2}
$n(\nu)$	$\frac{1}{2}$	2
$T(\nu)/\nu$	3	0

Table 3.6 Numerical results of the kinetic energy of localization, $T(\nu)$, the logarithmic derivative of the exponent $b(\nu)$, $n(\nu)$, and of the adjustable parameter, y.

ν	y	$T(\nu)$	$n(\nu)$
$1x10^{3}$	1.1305x10	6.3907x10	1.8799
$6x10^{2}$	9.5399	4.5505x10	1.8590
$2x10^{2}$	6.6231	2.1933x10	1.8023
$1x10^{2}$	5.2621	1.3845x10	1.7568
6x10	4.4420	9.8659	1.7176
2x10	3.0866	4.7635	1.6153
1x10	2.4536	3.0100	1.5373
6	2.0718	2.1461	1.4731
2	1.4394	1.0359	1.3176
1	1.1429	$6.5311x10^{-1}$	1.2098
$6x10^{-1}$	$9.6336x10^{-1}$	$4.6403x10^{-1}$	1.1278
$2x10^{-1}$	$6.6369x10^{-1}$	$2.2024x10^{-1}$	$9.5183x10^{-1}$
$1x10^{-1}$	$5.2139x10^{-1}$	$1.3593x10^{-1}$	$8.4771x10^{-1}$
$6x10^{-2}$	$4.3431x10^{-1}$	$9.4313x10^{-2}$	$7.7764x10^{-1}$
$2x10^{-2}$	$2.8703x10^{-1}$	$4.1193x10^{-2}$	$6.5367x10^{-1}$
$1x10^{-2}$	$2.1671x10^{-1}$	$2.3482x10^{-2}$	$5.9734x10^{-1}$
$6x10^{-3}$	$1.7421x10^{-1}$	$1.5175x10^{-2}$	$5.6671x10^{-1}$
$2x10^{-3}$	$1.0576x10^{-1}$	$5.5929x10^{-3}$	$5.2681x10^{-1}$
$1x10^{-3}$	$7.6006x10^{-2}$	$2.8884x10^{-3}$	$5.1434x10^{-1}$

Table 3.7 Numerical results of the dimensionless functions, $a(\nu)$, $b(\nu)$, and of the adjustable parameter, y.

ν	y	$a(\nu)$	$b(\nu)$
$1x10^{3}$	1.1305x10	$3.0379x10^{8}$	$1.4489x10^{6}$
$6x10^{2}$	9.5399	$5.6903x10^{7}$	$5.5754x10^{5}$
$2x10^{2}$	6.6231	$1.6627x10^{6}$	$7.4500x10^{4}$
$1x10^{2}$	5.2621	$1.9008x10^{5}$	$2.1691x10^{4}$
6x10	4.4420	$3.9867x10^{4}$	$8.9291x10^{3}$
2x10	3.0866	$1.5719x10^{3}$	$1.4281x10^{3}$
1x10	2.4536	$2.2683x10^{2}$	$4.7866x10^{2}$
6	2.0718	5.7802x10	$2.2184x10^{2}$
2	1.4394	3.6975	4.7809x10
1	1.1429	$7.5404x10^{-1}$	1.9908x10
$6x10^{-1}$	$9.6336x10^{-1}$	$2.5164x10^{-1}$	1.0958x10
$2x10^{-1}$	$6.6369x10^{-1}$	$2.9270x10^{-2}$	3.4993
$1x10^{-1}$	$5.2139x10^{-1}$	$8.6133x10^{-3}$	1.8767
$6x10^{-2}$	$4.3431x10^{-1}$	$3.6977x10^{-3}$	1.2397
$2x10^{-2}$	$2.8703x10^{-1}$	$6.7551x10^{-4}$	$5.6686x10^{-1}$
$1x10^{-2}$	$2.1671x10^{-1}$	$2.4324x10^{-4}$	$3.6783x10^{-1}$
$6x10^{-3}$	$1.7421x10^{-1}$	$1.1587x10^{-4}$	$2.7334x10^{-1}$
$2x10^{-3}$	$1.0576x10^{-1}$	$2.3665x10^{-5}$	$1.5034x10^{-1}$
$1x10^{-3}$	$7.6006x10^{-2}$	$8.6447x10^{-6}$	$1.0484x10^{-1}$

Table 3.8 Numerical results of the functions σ_o^2 , σ_1^2 , and μ for each values of the energy, ν .

ν	σ_o^2	σ_1^2	μ
$1x10^3$	$7.8118x10^{-1}$	2.6039	$1.3619x10^3$
$6x10^2$	$7.4735x10^{-1}$	2.0884	$8.6373x10^2$
$2x10^2$	$6.6113x10^{-1}$	1.2591	$3.3569x10^2$
$1x10^2$	$5.9752x10^{-1}$	$8.9016x10^{-1}$	$1.9053x10^2$
6x10	$5.4667x10^{-1}$	$6.7796x10^{-1}$	$1.2780x10^2$
2x10	$4.2940x10^{-1}$	$3.5588x10^{-1}$	5.7669x10
1x10	$3.5361x10^{-1}$	$2.2548x10^{-1}$	3.6792x10
6	$2.9913x10^{-1}$	$1.5645x10^{-1}$	2.7233x10
2	$1.9278x10^{-1}$	$6.4639x10^{-2}$	1.5748x10
1	$1.3737x10^{-1}$	$3.4198x10^{-2}$	1.2042x10
$6x10^{-1}$	$1.0332x10^{-1}$	$2.0464x10^{-2}$	1.0299x10
$2x10^{-1}$	$5.0469x10^{-2}$	$5.8746x10^{-3}$	8.3267
$1x10^{-1}$	$2.9659x10^{-2}$	$2.3855x10^{-3}$	7.9545
$6x10^{-2}$	$1.9211x10^{-2}$	$1.1518x10^{-3}$	8.0327
$2x10^{-2}$	$6.6059x10^{-3}$	$1.9535x10^{-4}$	9.2635
$1x10^{-2}$	$3.0477x10^{-3}$	$5.4321x10^{-5}$	1.0986x10
$6x10^{-3}$	$1.6403x10^{-3}$	$1.9520x10^{-5}$	1.2909x10
$2x10^{-3}$	$3.8349x10^{-4}$	$1.7727x10^{-6}$	1.9799x10
$1x10^{-3}$	$1.4421x10^{-4}$	$3.5259x10^{-7}$	2.6963x10

Table 3.9 Numerical results of the density of states, $\rho(E)$ in unit of $(Q^3/E_Q\xi^2)$ for $\xi' = \xi/E_Q^2 = 0.05,\ 0.50,\ 5$, and 50 respectively.

ν	$\rho(E)$			
	$\xi' = 50$	$\xi' = 5$	$\xi' = 0.50$	$\xi' = 0.05$
1×10^{3}	0.0000	0.0000	0.0000	0.0000
6×10^{2}	0.0000	0.0000	0.0000	0.0000
2×10^{2}	0.0000	0.0000	0.0000	0.0000
1×10^{2}	0.0000	0.0000	0.0000	0.0000
6×10	6.6367×10^{-35}	0.0000	0.0000	0.0000
2×10	9.8677×10^{-4}	1.4943×10^{-59}	0.0000	0.0000
1×10	1.8919	3.6947×10^{-19}	0.0000	0.0000
6	6.2879	1.3414×10^{-8}	0.0000	0.0000
2	2.2923	3.1016×10^{-2}	6.3788×10^{-21}	0.0000
1	6.1793×10^{-1}	1.0299×10^{-1}	1.7047×10^{-9}	0.0000
6×10^{-1}	2.2552×10^{-1}	8.4115×10^{-2}	4.3823×10^{-6}	6.4564×10^{-49}
2×10^{-1}	2.8264×10^{-2}	2.0628×10^{-2}	8.8454×10^{-4}	1.8592×10^{-17}
1×10^{-1}	8.4531×10^{-3}	7.1395×10^{-3}	1.3187×10^{-3}	6.0930×10^{-11}
6×10^{-2}	3.6521×10^{-3}	3.2666×10^{-3}	1.0705×10^{-3}	$1.5299\times10^{-}$
2×10^{-2}	6.7169×10^{-4}	6.3828×10^{-4}	3.8322×10^{-4}	2.3323×10^{-6}
1×10^{-2}	2.4234×10^{-4}	2.3445×10^{-4}	1.6838×10^{-4}	6.1455×10^{-6}
6×10^{-3}	1.1555×10^{-4}	1.1275×10^{-4}	8.8157×10^{-5}	7.5313×10^{-6}
2×10^{-3}	2.3629×10^{-5}	2.3312×10^{-5}	2.0362×10^{-5}	5.2625×10^{-6}
1×10^{-3}	8.6357×10^{-6}	8.5546×10^{-6}	7.7843×10^{-6}	3.0298×10^{-6}

3.2 Gaussian Potential

3.2.1 Present Method

The process of obtaining the density of states $\rho(E)$ for the case of Gaussian impurity potential is similar to the case of screened Coulomb potential. The only difference is that for the case of Gaussian impurity potential, the density of states can be conveniently evaluated by considering in the cartesian coordinates,

First starting from (2.1.46)

$$\theta - \mu\sigma_o^2 = E \qquad (3.2.1)$$

θ and σ_o^2 are given by (3.2.2) and (3.2.3) respectively

$$\theta = \int f(\vec{x}) \; T \; f(\vec{x}) d\vec{x} \qquad (3.2.2)$$

and

$$\sigma_o^2 = \int [f(\vec{x})]^2 \; U(\vec{x}) d\vec{x} \qquad (3.2.3)$$

The operator T is the kinetic energy of particle which has the simple form in unit of $\hbar^2/2m$

$$T = -\nabla^2 + E_o$$

or

$$T = -\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + E_o \qquad (3.2.4)$$

and the effective potential

$$U(\vec{x}) = \int [f(\vec{x}')]^2 \, W(\vec{x} - \vec{x}')d\vec{x} \qquad (3.2.5)$$

The correlation function $W(\vec{x}-\vec{x}')$ defined by (2.1.33) clearly depends on the impurity potential employed. For a Gaussian impurity potential, it is in the form

$$v(\vec{x}-\vec{R}) = u(\pi\ell^2)^{-3/2} \exp\left[-|\vec{x}-\vec{R}|^2/\ell^2\right] \qquad (3.2.6)$$

and it follows from (2.1.23) that

$$W(\vec{x}-\vec{x}') = u^2(\pi\ell^2)^{-3} \int_{-\infty}^{\infty} e^{(-|\vec{x}-\vec{R}|/\ell^2)} \, e^{(-|\vec{x}'-\vec{R}|/\ell^2)} \, d\vec{R} \qquad (3.2.7)$$

By using the formula

$$\int_{-\infty}^{\infty} e^{a(x_1-x)^2} \, e^{b(x_2-x)^2} \, dx = \left[-\frac{\pi}{(a+b)}\right]^{d/2} \exp\left[\frac{ab(x_1-x_2)^2}{(a+b)}\right] \qquad (3.2.8)$$

where d is dimensionality and here d = 3. Then an analytical expression of $W(\vec{x}-\vec{x}')$ is

$$W(\vec{x}-\vec{x}') = u^2(\pi L^2)^{-3/2} \exp[-|\vec{x}-\vec{x}'|^2/L^2] \qquad (3.2.9)$$

where L denotes the correlation length of the random system related to ℓ by the relation $L^2 = 2\ell^2$ and u is another parameter introduced in order to take care of the dimension of the system.

Assuming the trial wave function which satisfying (3.2.1) is the Gaussian ground-states wave function.

$$f(\vec{x}) = (2\xi_o/\pi)^{3/4} \exp(-\xi_o\vec{x}^2) \qquad (3.2.10)$$

where $\vec{x}^2 = x^2 + y^2 + z^2$ and $\xi_o = m\omega/2\hbar$ is a parameter to be determined. The wave function $f(\vec{x})$ obeys the normalization condition

$$\int_{-\infty}^{\infty}[f(\vec{x})]^2 d\vec{x} = (2\xi_o/\pi)^{3/2} \int_{-\infty}^{\infty} \exp[-2\xi_o\vec{x}^2]d\vec{x}$$

It is more convenient to use spherical polar coordinate to evaluate the above integral

$$\int_{-\infty}^{\infty}[f(\vec{x})]^2 d\vec{x} = (2\xi_o/\pi)^{3/2} 4\pi \int_{0}^{\infty} r^2 \exp(-2\xi_o r^2)dr$$

apply the formula

$$\int_{\infty}^{\infty} x^m \exp(-ax^2)\, d\vec{x} = \frac{\Gamma[(m+1)/2]}{2(a)^{(m+1)/2}}$$

where the gamma function $\Gamma(n+1) = n\Gamma(n)$ and $\Gamma(1/2) = \sqrt{\pi}$.

One gets

$$\int_{-\infty}^{\infty} [f(\vec{x})]^2 \, d\vec{x} = (2\xi_o/\pi)^{3/2} \left[\frac{4\pi\Gamma(3/2)}{2(2\xi_o)^{3/2}} \right] = 1 \qquad (3.2.12)$$

Once the trial wave function has been introduced, the function θ and σ_o^2 can be determined by operating the operator T on the wave function

$$Tf(\vec{x}) = [-(4\xi_o^2\vec{x}^2 - 6\xi_o) + E_o](2\xi_o/\pi)^{3/4} \exp(-\xi_o\vec{x}^2), \qquad (3.2.13)$$

and then substituting into (3.2.2) and using (3.2.12)

$$\theta = -(2\xi_o/\pi)^{3/2} \left[4\xi_o^2 \int_{-\infty}^{\infty} \vec{x}^2 \exp(-2\xi_o\vec{x}^2)\, d\vec{x} - 6\xi_o \int_{-\infty}^{\infty} \exp(-2\xi_o\vec{x}^2)\, d\vec{x} \right] + E_o$$

$$= -(2\xi_o/\pi)^{3/2} \left[16\pi\xi_o^2 \int_0^{\infty} r^4 \exp(-2\xi_o r^2)\, dr - 24\pi\xi_o \int_0^{\infty} r^2 \exp(-2\xi_o r^2)\, dr \right] + E_o$$

$$= 3\xi_o + E_o \qquad (3.2.14)$$

To evaluate σ_o^2 the function $U(\vec{x})$ must be known. From (3.2.9) and (3.2.10) $U(\vec{x})$ can be expressed as

$$U(\vec{x}) = (2\xi_o/\pi)^{3/2}[u^2/(\pi L^2)^{3/2}] \int_{-\infty}^{\infty} e^{-2\xi_o|\vec{b}-\vec{x}'|^2} e^{[-|\vec{x}-\vec{x}'|^2/L^2]} d\vec{x}'$$

$$= (2\xi_o/\pi)^{3/2}[u^2/(\pi L^2)^{3/2}][\pi L^2/(2\xi_o L^2+1)]^{3/2}\exp[-2\xi_o\vec{x}^2/(2\xi_o L^2+1)]$$

or

$$U(\vec{x}) = (K/\pi)^{3/2}\, u^2 \exp[-K\vec{x}^2] \qquad (3.2.15)$$

where $K = 2\xi_o/(2\xi_o L^2+1)$. Substituting (3.2.10) and (3.2.15) into (3.2.3), gives

$$\sigma_o^2 = (2\xi_o K/\pi^2)^{3/2}\, u^2 \int_{-\infty}^{\infty} \exp[-(2\xi_o + K)\vec{x}^2]\, d\vec{x}$$

$$= (2\xi_o K/\pi^2)^{3/2}\, 4\pi u^2 \int_{o}^{\infty} r^2 \exp[-(2\xi_o+K)r^2]\, dr$$

expressing K in terms of ξ_o , one gets

$$\sigma_o^2 = (u^2/\pi^{3/2})\,[\xi_o/(\xi_o L^2+1)]^{3/2} \qquad (3.2.16)$$

Combining the results for θ and σ_o^2 and putting into (3.2.1)

$$3\xi_o + E_o - \mu(u^2/\pi^{3/2})\,[\,\xi_o/(\xi_o L^2+1)\,]^{3/2} = E \qquad (3.2.17)$$

then

$$\mu = (\pi^{3/2}/u^2)\,[\,(E_o-E\,) + 3\xi_o\,]\,[\,(\xi_o L^2+1)/\,\xi_o\,]^{3/2}$$

or

$$\mu = (\pi^{3/2}u^2)\,(\nu E_L + 3\xi_o)\,[\,(\xi_o L^2+1)/\xi_o\,]^{3/2} \qquad (3.2.18)$$

where $\nu = (E_o - E\,)/E_L$ and $E_L = \hbar^2/2mL^2$.

Now σ_1^2 can be calculated as below

$$\sigma_1^2 = (-u^2/3)\,(2\xi_o K/\pi^2)^{3/2}\int_{-\infty}^{\infty}(-12\xi_o+16\xi_o^2\vec{x}^2)\exp[\,-(2\xi_o+K)\,\vec{x}^2\,]\,d\vec{x}$$

$$= (u^2/3)\,(2\xi_o K/\pi^2)^{3/2}[\;48\pi\,\xi_o\int_0^{\infty} r^2\,\exp\,-(2\xi_o+K)\,r^2\,dr$$

$$-\,64\,\pi\xi_o^2\int_0^{\infty} r^4\exp[\,-(2\xi_o+K)\,r^2\,]\,dr\,]$$

Using (3.2.11) and the relation $K = 2\xi_o/(2\xi_o L^2+1)$, one has

$$\sigma_1^2 = (2u^2/\pi^{3/2})\,[\,\xi_o/(\xi_o L^2+1)\,]^{5/2} \qquad (3.2.19)$$

Since $f(\vec{x})$ is spherically symmetric which means $\sigma_1^2 = \sigma_2^2 = \sigma_3^2$

and using the relation $\mu\sigma_o^2 = (\theta - E)$. The functions $A(E)$ and $B(E)$ can be written as

$$A(E) = \frac{\mu^3\sigma_1^3}{(2\pi)^2\sigma_o} = \frac{1}{\sqrt{2}\pi^2}\left(\frac{\pi}{u^2}\right)^{3/2}(\nu E_L + 3\xi_o)^3 [(\xi_o L^2+1)/\xi_o]^{3/2} \tag{3.2.20}$$

and

$$B(E) = \mu^2\sigma_o^2 = (\pi^{3/2}/u^2)(\nu E_L + 3\xi_o)^2 [(\xi_o L^2+1)/\xi_o]^{3/2} \tag{3.2.21}$$

Now the density of states can be written in the simple form as

$$\rho(E) = [(E_L/L)^3/\xi_L^2]\ a(\nu,z)\ \exp[-E_L^2\, b(\nu, z)/2\xi_L], \tag{3.2.22}$$

where

$$a(\nu, z) = (3z/4 + \nu)^3(1 + 4/z)^{3/2}/\sqrt{2}\pi^2 \tag{3.2.23}$$

and

$$b(\nu, z) = (3z/4 + \nu)^2(1 + 4/z)^{3/2}$$

with ξ_L, defined by Sa-yakanit, related to ξ by the relation

$\xi_L = [u^2/(\pi L^2)^{3/2}]\xi$ and has the dimension of the energy square, the variational parameter $z = E\omega/E_L$ or $z = 4\xi_o/E_L$ where

$E\omega = \hbar\omega$ and $E_L = 1/L^2$ (in unit of $\hbar^2/2m^*$). To determine ξ_0, z must be chosen so as to maximize $\rho(E)$. Similar to the Halperin and Lax method the best choice of z is chose from the condition of maximizing the exponential factor of (3.2.22) , i e., from the condition

$$\frac{d}{dz} b(\nu, z) = 0 = \frac{d}{dz} \ln b(\nu, Z)$$

$$= \frac{d}{dz} \left[2\ln\left(\frac{3}{4} z + \nu\right) + \frac{3}{2} \ln\left(1 + \frac{4}{z}\right)\right]$$

$$0 = z^2 + z - 4\nu \qquad (3.2.24)$$

For the same reason which is given in Sa-yakanit theory, only the positive root of (3.2.24) is kept

$$z = \left[(1 + 16\nu)^{1/2} - 1\right]/2 \qquad (3.2.25)$$

If both numerator and denominator of (3.2.23) are multiplied by $(z + 4)^{3/2}$ and then using (3.2.24), one gets

$$a(\nu, z) = \left(\frac{3}{4} z + \nu\right)^3 \frac{(z + 4)^3}{(z^2+4z)^{3/2} (2\pi)^2}$$

$$= \frac{(3z/4 + \nu)^3 (z + 4)^3}{(4\nu-z+4z)^{3/2} (2\pi)^2}$$

$$= (3z/4 + \nu)^{3/2}(z + 4)^3/\ 8\sqrt{2}\pi^2 \qquad (3.2.26)$$

or

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

(3.2.27)

and

$$b(\nu) = [(1 + 16\nu)^{1/2}-1]^{1/2}[(1 + 16\nu)^{1/2} + 7]^{7/2}/2^8 \qquad (3.2.28)$$

Obviously the above two equations are equivalent to (2.2.28) and (2.2.29) in Sa-yakanit theory respectively, also the other functions such as $n(\nu)$, $T(\nu)$ and the limiting values for these functions.

$$n(\nu) = 32\nu/[(1 + 16\nu)^{1/2}-1][(1 + 16\nu)^{1/2} + 7] \qquad (3.2.29)$$

and

$$T(\nu) = (3/4)z = (3/8)[(1 + 16\nu)^{1/2}-1] \qquad (3.2.30)$$

The limiting values for both cases of ν are given in Table 3.10.

Table 3.10 The limiting values for the functions $a(\nu)$, $b(\nu)$, $n(\nu)$ and $T(\nu)$

	$\nu \ll 1$	$\nu \gg 1$
$a(\nu)$	$32\sqrt{2}\ \nu^{3/2}/\pi^2$	$\nu^3/\sqrt{2}\pi^2$
$b(\nu)$	$16\nu^{1/2}$	ν^2
$n(\nu)$	$\frac{1}{2}$	2
$T(\nu)/\nu$	3	0

The numerical results for these functions (computed by computer program presented in Appendix C) are given in Table 3.11 and 3.12

Table 3.11 Numerical results of the kinetic energy of localization, $T(\nu)$, the logarithmic derivative of the exponent $b(\nu)$, $n(\nu)$, and of the adjustable parameter, z.

ν	z	$T(\nu)$	$n(\nu)$
$1x10^{3}$	6.2748x10	4.7061	1.9101
$6x10^{2}$	4.8492x10	3.6369x10	1.8857
$2x10^{2}$	2.7789x10	2.0842x10	1.8112
$1x10^{2}$	1.9506x10	1.4629x10	1.7447
6x10	1.5000x10	1.1250x10	1.6842
2x10	8.4582	6.3436	1.5184
1x10	5.8443	4.3832	1.3905
6	4.4244	3.3183	1.2878
2	2.3723	1.7792	1.0584
1	1.5615	1.1712	$9.2116x10^{-1}$
$6x10^{-1}$	1.1279	$8.4591x10^{-1}$	$8.2993x10^{-1}$
$2x10^{-1}$	$5.2469x10^{-1}$	$3.9352x10^{-1}$	$6.7394x10^{-1}$
$1x10^{-1}$	$3.0623x10^{-1}$	$2.2967x10^{-1}$	$6.0667x10^{-1}$
$6x10^{-2}$	$2.0000x10^{-1}$	$1.5000x10^{-1}$	$5.7143x10^{-1}$
$2x10^{-2}$	$7.4456x10^{-2}$	$5.5842x10^{-2}$	$5.2741x10^{-1}$
$1x10^{-2}$	$3.8516x10^{-2}$	$2.8887x10^{-2}$	$5.1430x10^{-1}$
$6x10^{-3}$	$2.3450x10^{-2}$	$1.7587x10^{-2}$	$5.0872x10^{-1}$
$2x10^{-3}$	$7.9370x10^{-3}$	$5.9527x10^{-3}$	$5.0297x10^{-1}$
$1x10^{-3}$	$3.9841x10^{-3}$	$2.988x10^{-3}$	$5.0149x10^{-1}$

Table 3.12 Numerical results of the dimensionless functions, $a(\nu)$, $b(\nu)$, and of the variational parameter, z.

ν	z	$a(\nu)$	$b(\nu)$
$1x10^{3}$	$6.2748x10$	$9.0232x10^{7}$	$1.2028x10^{6}$
$6x10^{2}$	$4.8492x10$	$2.0794x10^{7}$	$4.5609x10^{5}$
$2x10^{2}$	$2.7789x10$	$9.4413x10^{5}$	$5.9672x10^{4}$
$1x10^{2}$	$1.9506x10$	$1.4275x10^{5}$	$1.7382x10^{4}$
$6x10$	$1.5000x10$	$3.6943x10^{4}$	$7.2370x10^{3}$
$2x10$	8.4582	$2.3414x10^{3}$	$1.2405x10^{3}$
$1x10$	5.8443	$4.660x10^{2}$	$4.5226x10^{2}$
6	4.4244	$1.5231x10^{2}$	$2.2814x10^{2}$
2	2.3723	$1.7025x10$	$6.2877x10$
1	1.5615	4.9286	$3.1684x10$
$6x10^{-1}$	1.1279	2.0995	$2.0267x10$
$2x10^{-1}$	$5.2469x10^{-1}$	$3.7933x10^{-1}$	8.9206
$1x10^{-1}$	$3.0623x10^{-1}$	$1.3536x10^{-1}$	5.7311
$6x10^{-2}$	$2.0000x10^{-1}$	$6.3851x10^{-2}$	4.2439
$2x10^{-2}$	$7.4456x10^{-2}$	$1.2652x10^{-2}$	2.3285
$1x10^{-2}$	$3.8516x10^{-2}$	$4.5235x10^{-3}$	1.6236
$6x10^{-3}$	$2.3450x10^{-2}$	$2.1131x10^{-3}$	1.2504
$2x10^{-3}$	$7.9370x10^{-3}$	$4.0892x10^{-4}$	$7.1768x10^{-1}$
$1x10^{-3}$	$3.9841x10^{-3}$	$1.4478x10^{-4}$	$5.0672x10^{-1}$