CHAPTER IV

CONCLUSION AND DISCUSSION

4.1 Conclusion

In chapter II, the quantum mechanical methods used to find the density of states in heavily doped semiconductors are introduced. First Halperin and Lax use the minimum counting method which is based on the full quantum theory of Schrödinger. The method assumes that all the eigenstates of a given energy have the same shape, or equivalently, that all the corresponding potential wells have the same shape. The density of states deep in the tail is calculated by counting the number of wells having a particular ground state energy. The best ground state wave function $f(\vec{x})$ is obtained by maximizing the density of states. This procedure leads to an equation

$$Tf(\vec{x}) - \mu\, f(\vec{x}) \int [\, f(\vec{x}')\,]^2 \; w(\vec{x}-\vec{x}') \;\; d\vec{x}' = Ef(\vec{x}) \qquad (4.1.1)$$

which looks like the Hartree equation for a particle bound in its own self-consistent field, with an interaction $-\mu w(\vec{x}-\vec{x}')$. The difference between this equation and the Hartree equation is that μ instead of E plays the role of the eigenvalue to be found. Using the technique developed by Hartree for solving the self-consistent equation[38],

Halperin and Lax have calculated the above equation numerically. The results are presented in the form of numerical functions for $a(\nu)$, $b(\nu)$, $n(\nu)$, and $T(\nu)$. Secondly, Sa-yakanit has used the Feynman path integral technique to acheive an analytical form of density of states. Because the density of states per unit volume is expressed in terms of the diagonal part of the average propagator, $G(\vec{x}_2, \vec{x}_1, t)$; to obtain the density of states, one has to find an approximate expression for G. To do this he approximated the action S by a nonlocal harmonic trial action S_o which contains an unknown parameter to be determined. After the process of calculation, the density of states deep in the tail can be expressed in analytical forms. For determining the unknown parameter introduced in the trial action S_o he followed Halperin and Lax method, i.e. he maximized the exponential factor of (2.2.23) and (2.2.46)

and obtained

$$x^2 + x - 4\nu = 0 \qquad\qquad (4.1.2)$$

for the Gaussian impurity potential, and

$$D_{-3}(z) = \frac{z^3}{2}(\frac{3}{2}z^{-2} + \nu)\, D_{-4}(z) \qquad\qquad (4.1.3)$$

for the screened Coulomb potential.

The numerical results for the functions $a(\nu)$, $b(\nu)$, $n(\nu)$, and $T(\nu)$ for a screened Coulomb potential obtained from Sa-yakanit theory can be compared with the numerical calculation by Halperin and Lax. But for a Gaussian impurity potential (in three dimensions) no such comparison can be made because no result calculated from the minimum counting method is available. Therefore, in this thesis special attention is given to evaluate the density of states for the case of Gaussian impurity potential by using the minimum counting method. Although it can be calculated numerically as was done by Halperin and Lax **but** the process of calculation is cumbersome since it involves the Hartree-type equation.

In chapter III, the simplified method is presented. The simply guessed initial wave functions are **used** **in** **the** expressions **of** Halperin and Lax theory. Analytical expressions of density of states tail are easily obtained. This method is not only the simple method but also gives the excellent results. The important point of this method is the guessing of an appropriated trial wave function .

4.2 Comparison of Results

4.2.1 Screened Coulomb Potential

For screened Coulomb potential, the results of Eymard and Duraffourg method can be improved by using the trial wave function in the form

$$\phi(r) = (2\beta^4/3\pi)^{1/2} r^{1/2} \exp(-\beta r) \qquad (4.1.4)$$

An analytical expression of the density of states is easily obtained

$$\rho(E) = \left[(E_Q Q)^3/\xi^2 \right] a(\nu) \exp\left[-E_Q^2 b(\nu)/2\xi \right] \qquad (4.1.5)$$

where

$$a(\nu) = \frac{546(2\nu+y^2)^3(2y+1)^{14}(264y^3+60y^2+14y+1)^{3/2}}{(27)^{3/2}\pi^2 y^3(1152y^4+728y^3+244y^2+42y+3)^{7/2}} \qquad (4.1.6)$$

and

$$b(\nu) = \frac{9}{4}\frac{(2\nu+y^2)^2(2y+1)}{y^3(1152y^4+728y^3+244y^2+42y+3)} \qquad (4.1.7)$$

The comparison of the numerical results for the dimensionless functions $a(\nu)$ and $b(\nu)$, and for the limiting values of $a(\nu)$, $b(\nu)$, $n(\nu)$, and $T(\nu)/\nu$ obtained from Halperin and Lax theory,

Sa-yakanit theory, Eymard and Duraffourg, and Present method is presented in Table 4.1 , 4.2, and 4.3 respectively. The density of states calculated from the four methods are plotted in the same figure, such as Fig. 4.1 to 4.4 for $\xi' = 0.05, 0.5, 5$ and 50 respectively. The function $n(\nu)$ is plotted in Fig. 4.5.

It can be seen from Table 4.1 - 4.3 and from Fig. 4.1 - 4.4 that the results of present method are in very good agreement with the computed Halperin and Lax results. Especially, for the large values of ν the function $a(\nu)$ and $b(\nu)$ obtained from present method are closer to Halperin and Lax's results than those obtained from Eymard and Duraffourg method. For the large values of ξ' (for example $\xi' = 50$) the density of states calculated by present method also gives the better results than those calculated by the method of Eymard and Duraffourg. But for small values of ξ' (for example $\xi' = 0.05$) present method yeilds the smaller value of $\rho_1(E)$ than Eymard and Duraffourg method and than Halperin and Lax theory. From Table 4.3 it is interesting to note that present method, Eymard and Duraffourg method, Sa-yakanit theory, and Halperin and Lax theory predict identical limiting values for $n(\nu)$ and $T(\nu)/\nu$ but slightly different values for $a(\nu)$ and $b(\nu)$. From Fig 4.5, as $\nu \longrightarrow \infty$ and $\nu \longrightarrow 0$ the values of $n(\nu)$ obtained from the four methods tend to 2 and $\frac{1}{2}$ respectively. This result agrees with the experimental results.

Table 4.1 Comparison between the value of $a(\nu)$ calculated from the present
method, Eymard and Duraffourg method, Sa-yakanit Theory and
Halperin and Lax Theory for the case of a screened Coulomb potential.

ν	$a(\nu)$			
	PRESENT METHOD	EYMARD-DURAFFOURG METHOD	SA-YAKANIT THEORY	HALPERIN AND LAX THEORY
1.000×10^3	3.0379×10^8	3.1209×10^8	2.9442×10^8	3.098×10^8
5.623×10^2	4.6068×10^7	4.7703×10^7	4.4467×10^7	4.645×10^7
3.162×10^2	7.1629×10^6	7.4859×10^6	6.8822×10^6	7.250×10^6
1.778×10^2	1.1469×10^6	1.2118×10^6	1.0963×10^6	1.153×10^6
1.00×10^2	1.9008×10^5	2.0321×10^5	1.8063×10^5	1.888×10^5
5.623×10	3.2779×10^4	3.5525×10^4	3.0954×10^4	3.223×10^4
3.162×10	5.9174×10^3	6.5109×10^3	5.5499×10^3	5.781×10^3
1.778×10	1.1252×10^3	1.2588×10^3	1.0479×10^3	1.094×10^3
1.000×10	2.2683×10^2	2.5833×10^2	2.0975×10^2	2.197×10^2
5.623	4.8783×10	5.6617×10	4.4800×10	4.689×10
3.162	1.1257×10	1.3322×10	1.0273×10	1.078×10
1.778	2.8011	3.3813	2.5424	2.793
1.000	7.5404×10^{-1}	9.2839×10^{-1}	6.8151×10^{-1}	7.259×10^{-1}
5.623×10^{-1}	2.1991×10^{-1}	2.7609×10^{-1}	1.9817×10^{-1}	2.157×10^{-1}
3.162×10^{-1}	6.9419×10^{-2}	8.8843×10^{-2}	6.2444×10^{-2}	5.957×10^{-2}
1.778×10^{-1}	2.3627×10^{-2}	3.0826×10^{-2}	2.1232×10^{-2}	2.423×10^{-2}
1.000×10^{-1}	8.6132×10^{-3}	1.1464×10^{-2}	7.7327×10^{-3}	8.906×10^{-3}
5.623×10^{-2}	3.3312×10^{-3}	4.5307×10^{-3}	2.9851×10^{-3}	3.532×10^{-3}

Table 4.1 (Continued)

ν	a(ν)			
	PRESENT METHOD	EYMARD-DURAFFOURG	SA-YAKANIT THEORY	HALPERINAAND LAX THEORY
3.162×10^{-2}	1.3509×10^{-3}	1.8823×10^{-3}	1.2057×10^{-3}	1.485×10^{-3}
1.778×10^{-2}	5.6703×10^{-4}	8.1192×10^{-4}	5.0249×10^{-4}	5.407×10^{-4}
1.000×10^{-2}	2.4323×10^{-4}	3.5878×10^{-4}	2.1316×10^{-4}	2.834×10^{-4}
5.623×10^{-3}	1.0549×10^{-4}	1.6034×10^{-5}	9.1063×10^{-5}	1.290×10^{-5}
3.162×10^{-3}	4.5914×10^{-5}	7.1686×10^{-5}	3.8909×10^{-5}	5.890×10^{-5}
1.778×10^{-3}	1.9959×10^{-5}	3.1823×10^{-5}	1.6578×10^{-5}	
1.000×10^{-3}	8.6447×10^{-6}	1.3976×10^{-5}	7.0408×10^{-6}	

Table 4.2 Comparison between the value of $b(\nu)$ calculated from the present method, Eymard and Duraffourg method, Sa-yakanit Theory and Halperin and Lax Theory for the case of a screened Coulomb potential.

ν	$b(\nu)$			
	PRESENT METHOD	EYMARD AND DURAFFOURG METHOD	SA-YAKANIT THEORY	HALPERIN AND LAX THEORY
1.00×10^3	1.4489×10^6	1.4743×10^6	1.4378×10^6	1.444×10^6
5.623×10^2	4.9429×10^5	5.0454×10^5	4.8986×10^5	4.912×10^5
3.162×10^2	1.7114×10^5	1.7532×10^5	1.6938×10^5	1.702×10^5
1.778×10^2	6.0307×10^4	6.2025×10^4	5.9594×10^4	6.000×10^4
1.000×10^2	2.1690×10^4	2.2407×10^4	2.1401×10^4	2.150×10^4
5.623×10	7.9897×10^3	8.2931×10^3	7.8716×10^3	7.808×10^3
3.162×10	3.0252×10^3	3.1558×10^3	2.9765×10^3	2.988×10^3
1.778×10	1.1821×10^3	1.2393×10^3	1.1619×10^3	1.167×10^3
1.000×10	4.7866×10^2	5.0427×10^2	4.7030×10^2	4.716×10^2
5.632	2.0169×10^2	2.1339×10^2	1.9824×10^2	1.983×10^2
2.162	8.8797×10	9.4260×10	8.7403×10	8.720×10
1.778	4.0995×10	4.3598×10	4.0465×10	4.043×10
1.000	1.9907×10	2.1169×10	1.9736×10	1.956×10
5.632×10^{-1}	1.0189×10	1.0808×10	1.0163×10	1.008×10
3.162×10^{-1}	5.5017	5.8065	5.5301	5.456
1.778×10^{-1}	3.1324	3.2799	3.1776	3.108
1.000×10^{-1}	1.8766	1.9444	1.9232	1.846
5.632×10^{-2}	1.1789	1.2061	1.2210	1.151
3.162×10^{-2}	7.7275×10^{-1}	7.7958×10^{-1}	8.0860×10^{-1}	7.516×10^{-1}

Table 4.2 (Continued)

ν	b(ν)			
	PRESENT METHOD	EYMARD AND DURAFFOURG METHOD	SA-YAKANIT THEORY	HALPERIN AND LAX THEORY
1.778×10^{-2}	5.2529×10^{-1}	5.2238×10^{-1}	5.5482×10^{-1}	5.006×10^{-1}
1.000×10^{-2}	3.6783×10^{-1}	3.6086×10^{-1}	3.9159×10^{-1}	3.430×10^{-1}
5.632×10^{-3}	2.6351×10^{-1}	2.5549×10^{-1}	2.8228×10^{-1}	2.464×10^{-1}
3.162×10^{-3}	1.9191×10^{-1}	1.8433×10^{-1}	2.0652×10^{-1}	1.806×10^{-1}
1.778×10^{-3}	1.4133×10^{-1}	1.3483×10^{-1}	1.5258×10^{-1}	
1.000×10^{-3}	1.0484×10^{-1}	9.9557×10^{-2}	1.1342×10^{-1}	

Table 4.3 Comparison between the limiting values of $a(\nu)$, $b(\nu)$, $n(\nu)$, and $T(\nu)/\nu$ calculated from the present method, Eymard and Duraffourg method (ED), Sa-yakanit theory (VS) and Halperin and Lax Theory (HL) for the case of a screened Coulomb potential.

	$\nu \ll 1$				$\nu \gg 1$			
	PRESENT METHOD	ED METHOD	VS THEORY	HL THEORY	PRESENT METHOD	ED METHOD	VS THEORY	HL THEORY
$a(\nu)$	$0.29\nu^{3/2}$	$\approx 0.48\nu^{3/2}$	$\approx 0.23\nu^{3/2}$	$\approx 0.4\nu^{3/2}$	$\approx 0.42 \times 10^{-2}\nu^{7/2}$	$\approx 0.5 \times 10^{-2}\nu^{7/2}$	$\approx 0.5 \times 10^{-2}\nu^{7/2}$	$\approx 10^{-2}\nu$
$b(\nu)$	$3.26\nu^{1/2}$	$\approx 3.07\nu^{1/2}$	$\approx 3.54\nu^{1/2}$	$\approx 3\nu^{1/2}$	$\approx \nu^2$	$\approx \nu^2$	$\approx \nu^2$	$\approx \nu$
$n(\nu)$	$\approx \frac{1}{2}$	$\approx \frac{1}{2}$	$\approx \frac{1}{2}$	$\approx \frac{1}{2}$	≈ 2	≈ 2	≈ 2	≈ 2
$T(\nu)/\nu$	≈ 3	≈ 3	≈ 3	≈ 3	≈ 0	≈ 0	≈ 0	≈ 0

Left figure:

PRESENT METHOD
------ EYMARD AND DURAFFOURG METHOD
-·-·- HALPERIN AND LAX THEORY
×-×-×-× SA-YAKANIT THEORY

$\xi' = 100$

$\rho(E)$

ν

Fig 4.1 The density of states $\rho(E)$, in the dimensionless
form, $a(\nu) \exp[-b(\nu)/2\xi']$, is plotted against ν
for $\xi' = 100$

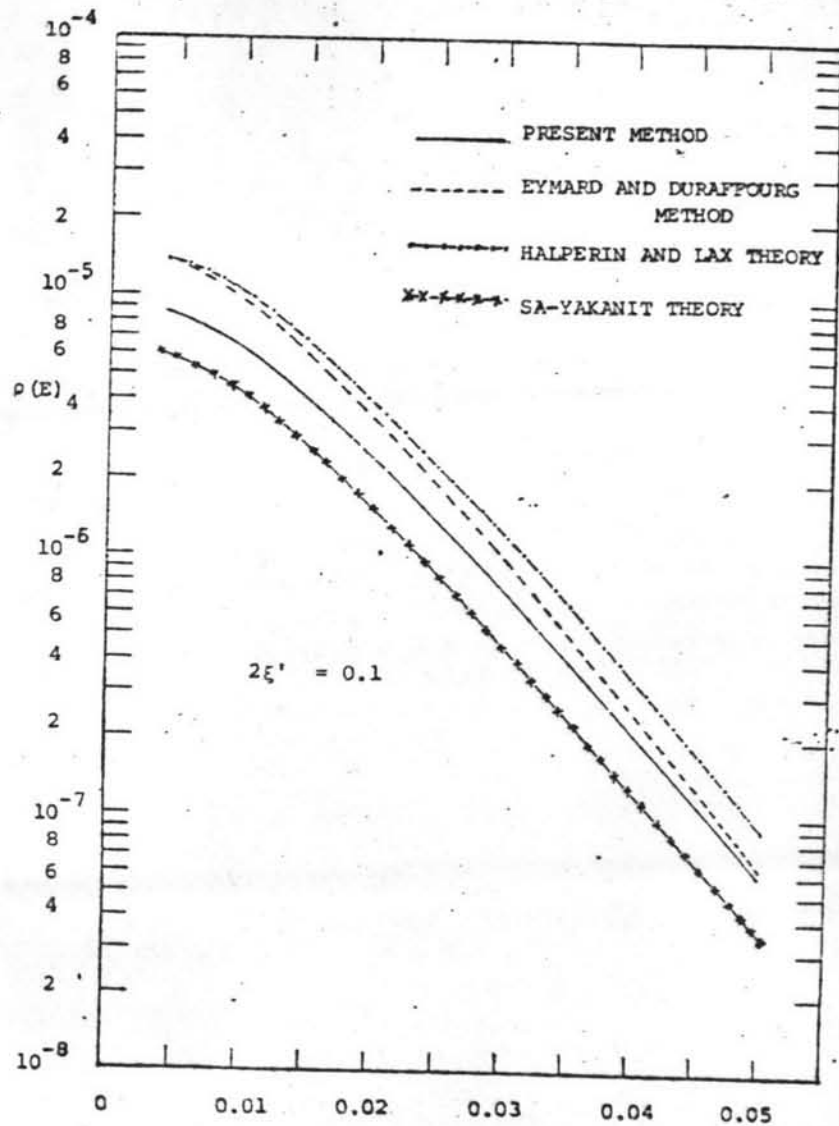**Right figure:**

—— PRESENT METHOD
------ EYMARD AND DURAFFOURG
METHOD
·-·-· HALPERIN AND LAX THEORY
×-×-×-× SA-YAKANIT THEORY

$2\xi' = 10$

$\rho(E)$

ν

Fig. 4.2 The density of states $\rho(E)$, in the dimensionless form,
$a(\nu) \exp[-b(\nu)/2\xi']$, is plotted against ν for $\xi' =$

Left plot:

PRESENT METHOD

EYMARD AND DURAFFOURG METHOD

HALPERIN AND LAX THEORY

SA-YAKANIT THEORY

$2\xi' = 1$

$b(E)$

Fig. 4.3   The density of states $\rho(E)$, in the dimensionless form,

$a(\nu) \exp[-b(\nu)/2\xi']$ is plotted against ν for $\xi' = 1$

Right plot:

PRESENT METHOD

EYMARD AND DURAFFOURG METHOD

HALPERIN AND LAX THEORY

SA-YAKANIT THEORY

$2\xi' = 0.1$

$\rho(E)$

Fig. 4.4 The density of states $\rho(E)$, in the dimensionle

form, $a(\nu) \exp[-b(\nu)/2\xi']$ is plotted against

for $\xi' = 0.1$
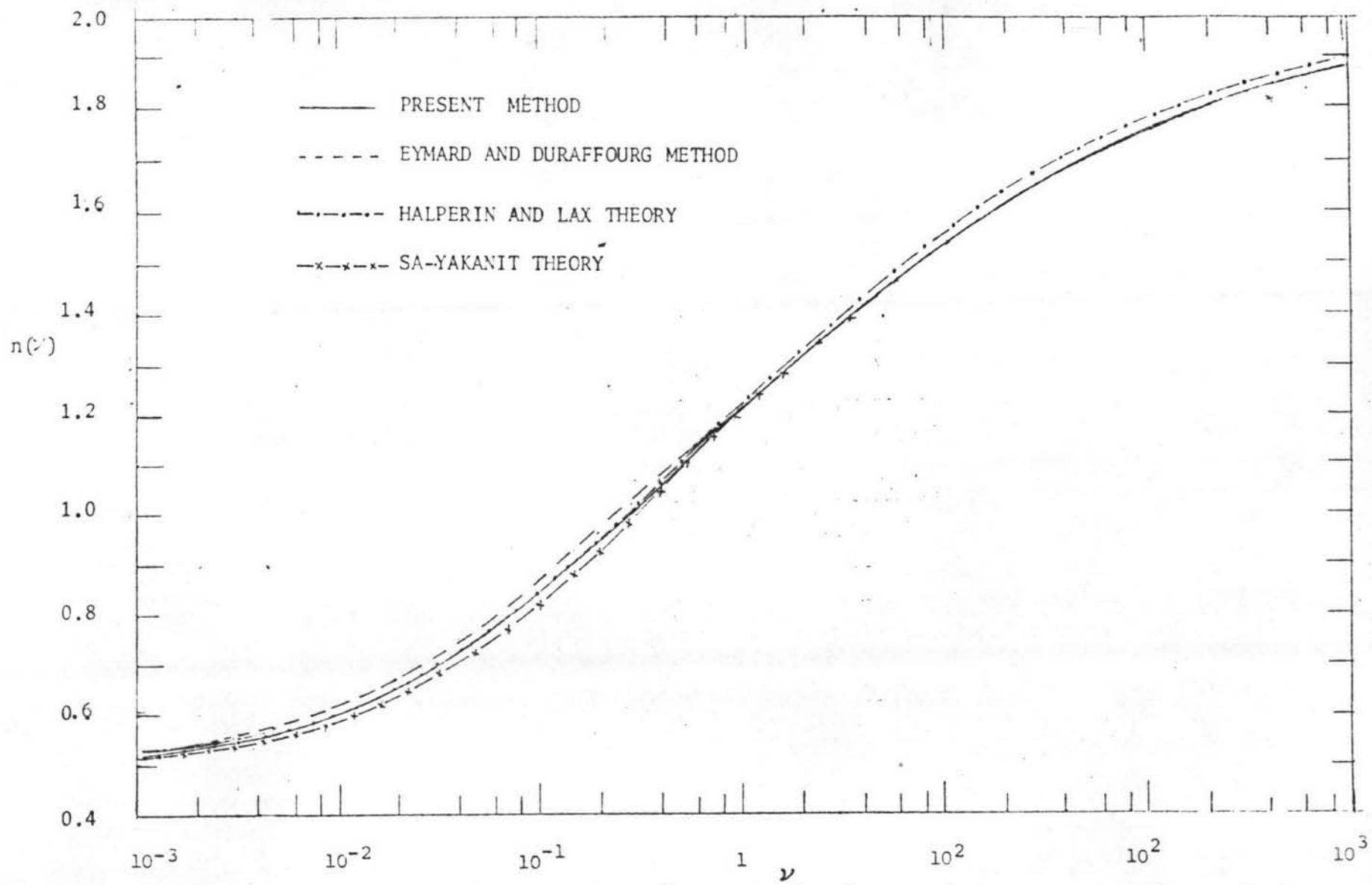
Fig. 4.5 The logarithmic derivative $n(\nu) = [d \log b(\nu)] / [d \log \nu]$ obtained from four methods are plotted against the energy ν.

Since the Hydrogen-like wave function and the present wave function,

$\phi(r) = (2\beta^4/3\pi)^{1/2} r^{1/2} \exp(-\beta r)$ give the better results in

different range of ξ' then their linear combination,

$\phi(r) = C_1 \exp(-\alpha r) + C_2 r^{1/2} \exp(-\beta r)$ might give the better results

for all range of ξ'. But the calculation would be very tedious.

The other interesting point is the variational condition.
For very small values of ν, and therefore $b(\nu)$, the exponential
factor of $\rho_1(E)$ is not dominate. The correct procedure consists in
maximizing $a(\nu) \exp[-E_Q^2 b(\nu)/2\xi]$ instead of minimizing $b(\nu)$ alone.
The results of this calculation are fortunately not very different from
those given above[31]. The variational condition can be written :

$$0 = y^2(4561920y^8 + 3080832y^7 + 1641024y^6 + 586360y^5 + 145764y^4 + 25314y^3$$

$$+ 3191y^2 + 270y + 9) - 2\nu(1824768y^8 + 4024128y^7 + 2235168y^6 + 776189y^5 +$$

$$+ 183264y^4 + 31764y^3 + 3826y^2 + 270y + 9) - \frac{9}{8\xi} \cdot \left[(2\nu + y^2)^2 (2y+1)^7 (264y^3 + 60y^2 + 14y \right.$$

$$\left. [y^2(9216y^5 + 3828y^4 + 1472y^3 + 344y^2 + 48y + 3) - 2\nu(6604y^4 + 3392y^3 + 968y^2 + 144y + 9) \right]$$

$$\left. (1152y^7 + 728y^6 + 244y^5 + 42y^4 + 3y^3) \right] \qquad (4.1.8)$$

which for $\nu \ll 1$ gives $y \simeq \sqrt{2}\, \nu^{1/2}$, $a(\nu) \simeq 0.2\nu^{3/2}$,
$b(\nu) \simeq 4.12\nu^{1/2}$, compare to those obtained by minimizing $b(\nu)$ alone

which are $y \simeq (6\nu)^{1/2}$, $a(\nu) \simeq 0.29\nu^{3/2}$, $b(\nu) \simeq 3.26\nu^{1/2}$. It seems that the improvement in accuracy with the exact calculation is not great enough to forbid the use of the very simple expressions derived from $\partial b/\partial y = 0$, since the asymptotic dependences have been shown to be the good ones.

The limiting of validity of present method is the same with Halperin and Lax theory, i.e., it is valid in the deep tail region due to considering only the ground state energy. And the results of present method are also in very good agreement with computed Halperin and Lax results. The systematic difference between Halperin and Lax's results and this work arises from the simplicity of an expression of the present wave function.

4.2.2 Gaussian Potential

For a Gaussian impurity potential, a ground state Gaussian wave function is tried.

$$f(\vec{x}) = (2\xi_0/\pi)^{3/4} \exp(-\xi_0 \vec{x}^2) \tag{4.1.9}$$

It is found that the density of states deep in tail can be expressed analytically as follows

$$\rho_1(E) = \left[(E_L/L)^3/\xi_L^2 \right] a(\nu) \exp\left[-E_L^2 b(\nu)/2\xi_L \right] \tag{4.1.10}$$

where

$$a(\nu) \;=\; [\,(1+16\nu)^{1/2}-1\,]^{3/2}\,[\,(1+16\nu)^{1/2}+7\,]^{9/2}\,/2^{12}\sqrt{2}\,\pi^2 \qquad (4.1.11)$$

and

$$b(\nu) \;=\; [\,(1+16\nu)^{1/2}-1\,]^{1/2}\,[\,(1+16\nu)^{1/2}+7\,]^{7/2}/2^{8} \qquad (4.1.12)$$

These expressions are equivalent to the expressions (2.2.28) and (2.2.29) derived by the path integral method. This means that for a Gaussian impurity potential, the results obtained from present method and Sa-yakanit theory are identical.

Obviously, the present method is more simple than Halperin and Lax theory. It gives the simple expressions which can be calculated by scientific calculator. The density of states for each values of ξ'_L are plotted on a semilog scale in Fig 4.6 to 4.9 and the function $n(\nu)$ is plotted on a log-log scale in Fig.4.10

Some advantages of present method for both screened Coulomb potential and Gaussian impurity potential are as follows: (i) The calculation can be performed analytically with simple integration by using simple trial wave functions (ii) The numerical results for the density of states are easily obtained because the solution of Hartree-Fock like eigenvalue equation is reduced to just solving the simple polynomial algebraic equations.
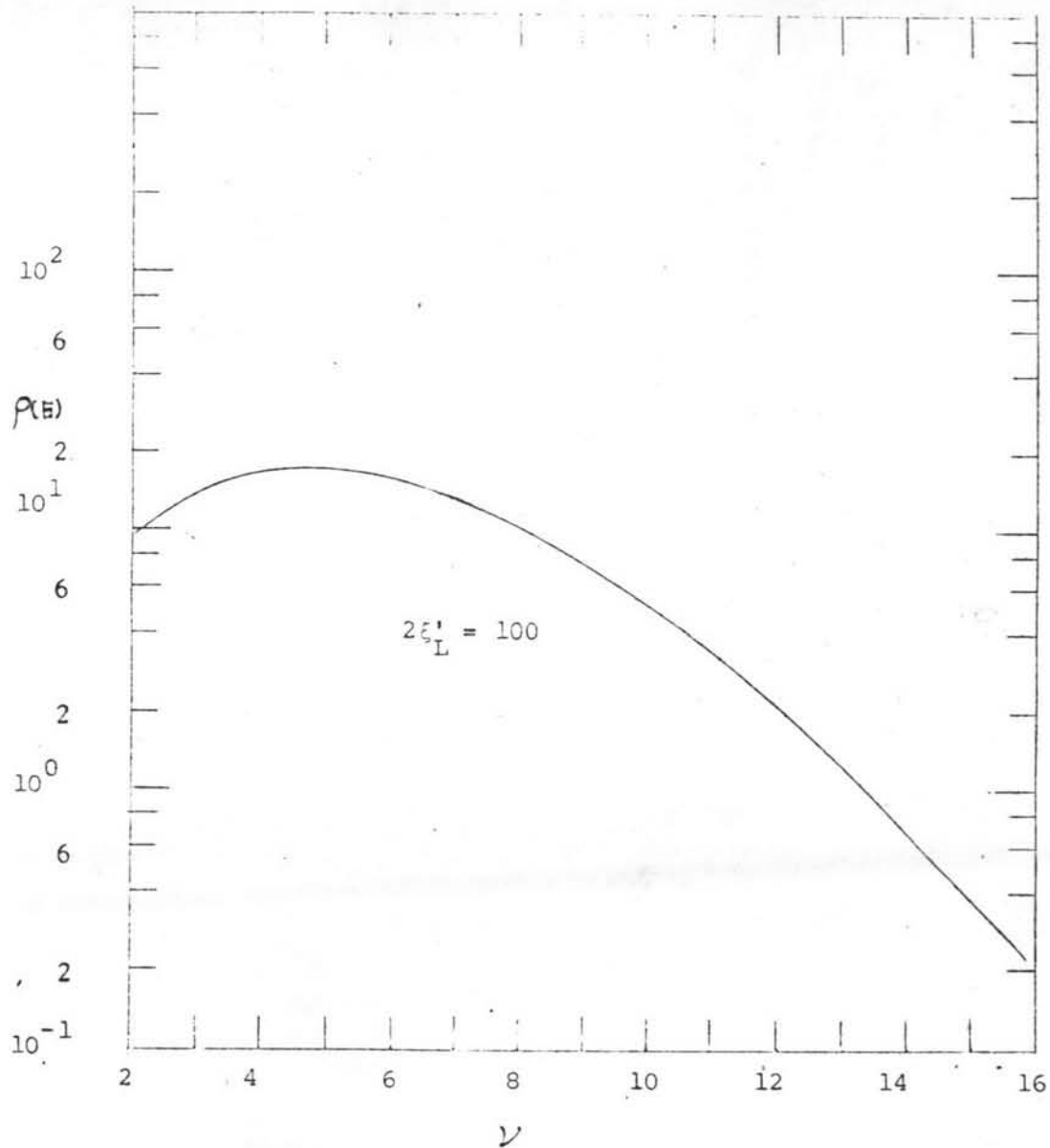
Fig.4.6 The density of states $\rho(E)$, in the dimensionless form, $a(\nu)\exp[-b(\nu)/2\xi_L']$ is plotted against for $\xi_L'=100$.
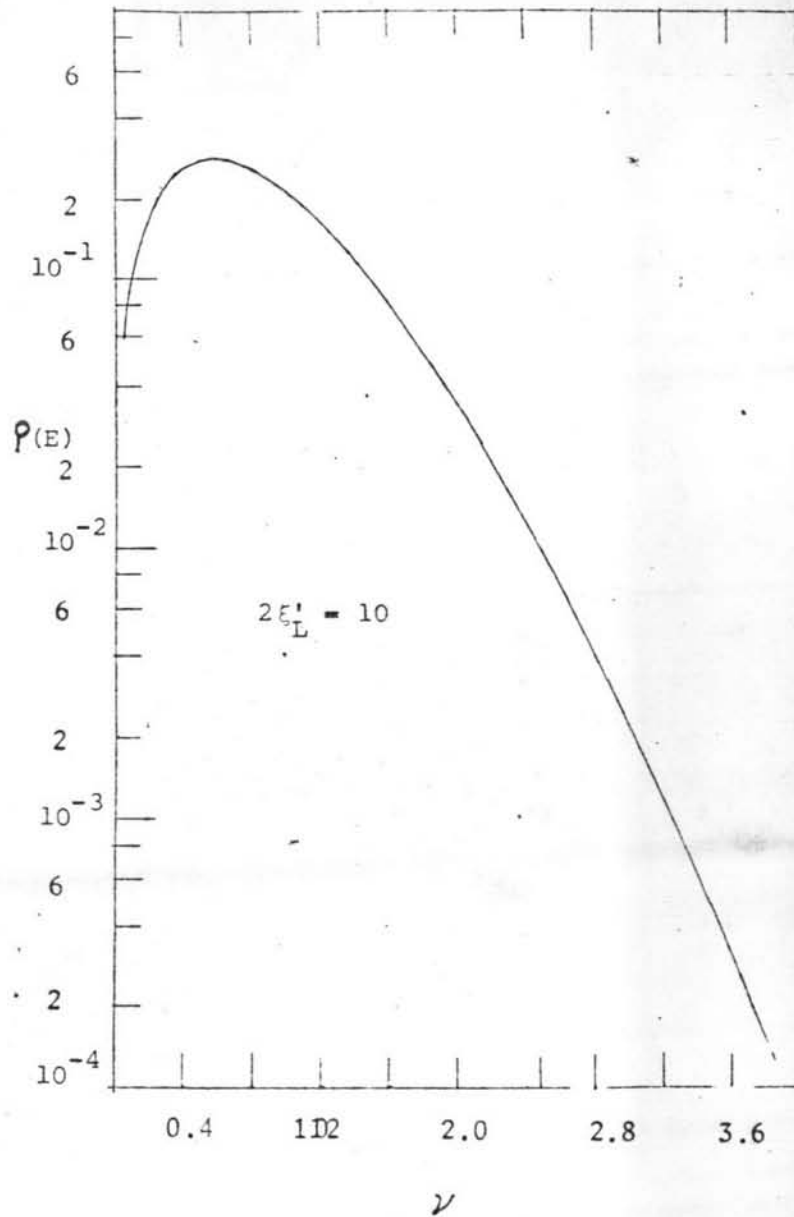
Fig.4.7 The density of states $\rho(E)$, in the dimensionless form $a(\nu)\exp[-b(\nu)/2\xi_L']$ is plotted against for $\xi_L'=10$.
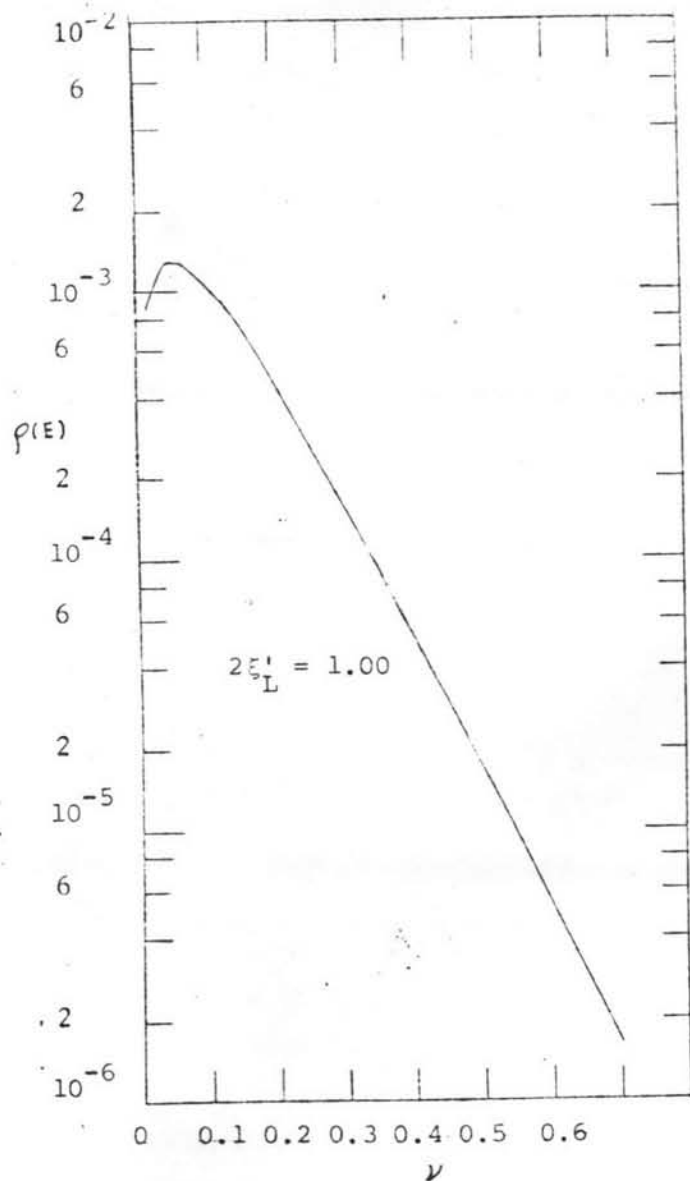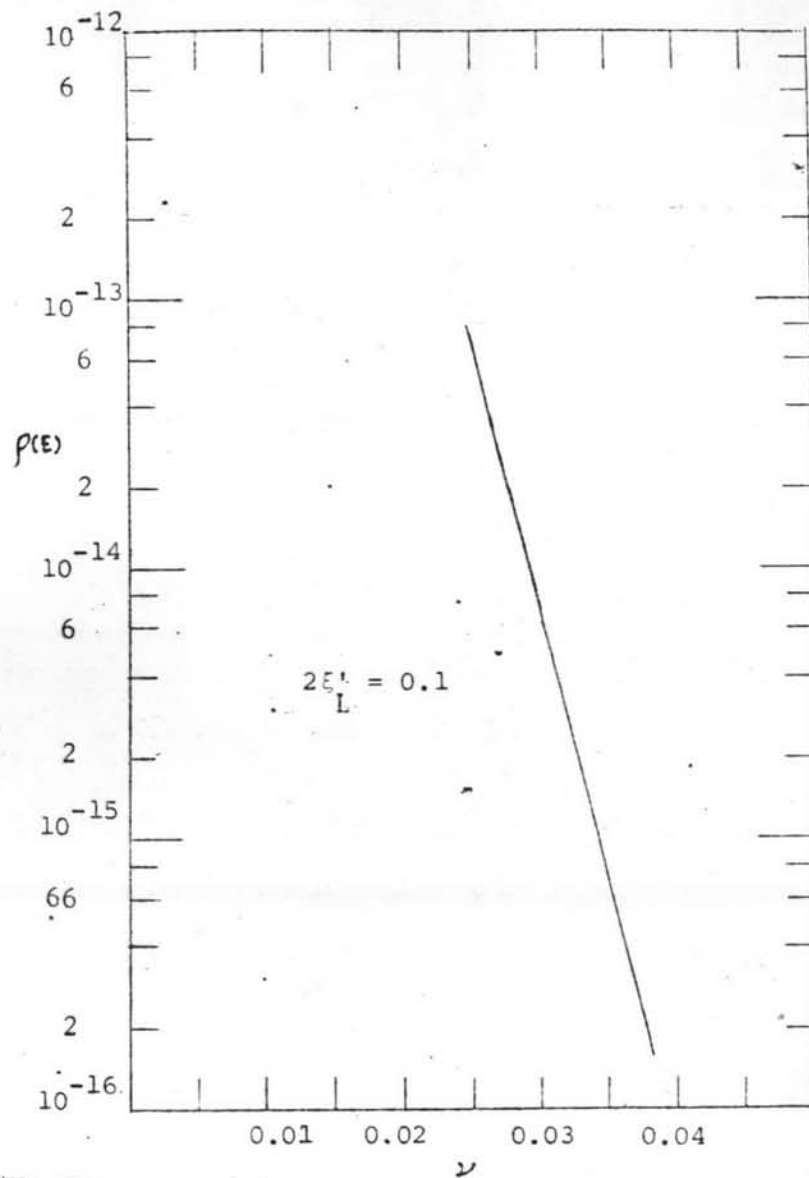
Fig. 4.8 The density of states $\rho(E)$, in the dimensionless form, $a(\nu)\ \exp\left[-b(\nu)/2\xi'_L\right]$ is plotted against ν for $\xi'_L = 1.00$.

Fig. 4.9 The density of states $\rho(E)$, in the dimensionless form, $a(\nu)\ \exp\left[-b(\nu)/2\xi'_L\right]$, is plotted against ν for $\xi'_L = 0.1$.
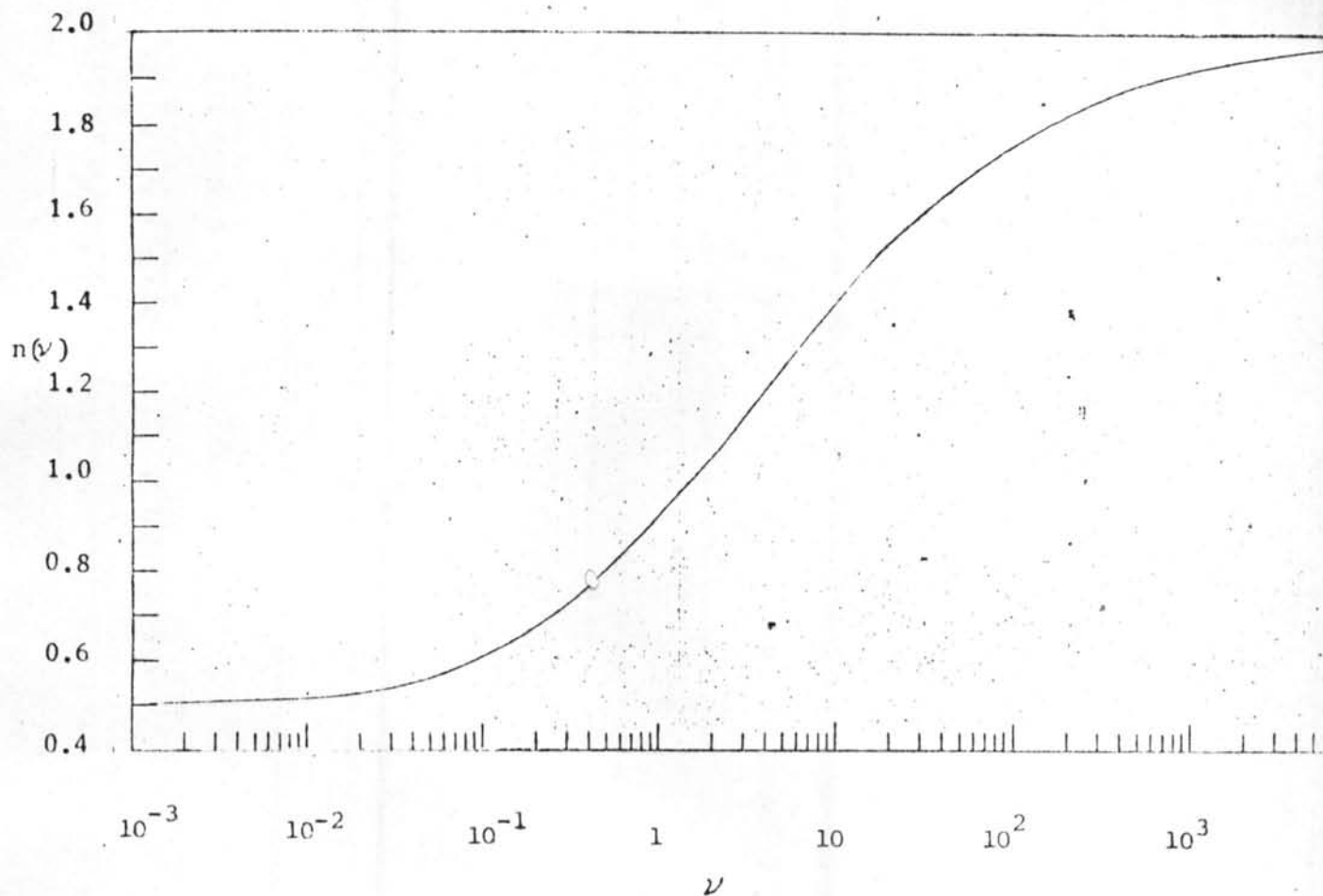
Fig. 4.10 The logarithmic derivative $n(\nu) = [d \log b(\nu)] / [d \log \nu]$ of the exponent $b(\nu)$ in the density of states is plotted and is shown to vary smoothly from $n(\nu) = \frac{1}{2}$ to 2.

4.2.3   The Application of the Impurity Potential Models.

For screened Coulomb potential the results can be used to study in heavily doped semiconductors.   The carrier screening length can be determined by using self-consistent method[38]   .   For a Gaussian potential the results can be used to study the noncrystalline structures such as poly-crystallines and amorphous semiconductors.   Since one usually does not know the detailed shape of the noncrystalline structure,   the autocorrelation length can be estimated from experiment.