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Electron density of states in a Gaussian random potential: Path-integral approach

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The behavior of the electron density of states in a Gaussian random potential is studied in the limit of low energies using the Feynman path-integral method. Two different impurity potentials are considered: the Gaussian potential and the screened Coulomb potential. It is shown that the density of states deep in the tail, in three dimensions, can be expressed analytically in the form proposed by Halperin and Lax, $\rho(E) = [A(E)/\xi^2]\exp[-B(E)/2\xi]$, where ξ is proportional to the density of impurities and to the square of the strength of the impurity potential. For a Gaussian potential with autocorrelation length L, we find $A(E) = (E_L/L)^3 a(\nu)$ and $B(E) = E_L^2 b(\nu)$, where $a(\nu) = [(1+16\nu)^{1/2}-1]^{3/2}[(1+16\nu)^{1/2}+7]^{9/2}/2^{12}2^{1/2}\pi^2$ and $b(\nu) = [(1+16\nu)^{1/2}-1]^{1/2}[(1+16\nu)^{1/2}+7]^{7/2}/2^8$, with ν being the energy below the mean potential E_0 in units of $E_L = \hbar^2/2mL^2$. For screened Coulomb potential with inverse screening length Q, we find $A(E) = (E_Q Q)^3 a(\nu,z)$ and $B(E) = E_Q^2 b(\nu,z)$ where $a(\nu,z) = (3/2z^2+\nu)^{3/2}/8\pi 2^{1/2} z^6 \exp(z^2/2) D_{-3}^2(z)$ and $b(\nu,z) = \pi^{1/2}(3/2z^2+\nu)^2/2^{3/2}\exp(z^2/4)D_{-3}(z)$, with z satisfying the equation $D_{-3}(z) = (z^3/2)(3/2z^2+\nu)D_{-4}(z)$, ν being the energy below the mean potential E_0 in units of $E_Q = \hbar^2 Q^2/2m$ and $D_p(z)$ denoting the parabolic cylinder function. Numerical results and calculated curves are presented. A detailed comparison with the minimum counting method of Halperin and Lax is given.

I. INTRODUCTION

In a previous paper,[1] we presented a method for calculating the density of states and the effective mass of an electron moving in a random system containing a high number of impurities, or equivalently, in a Gaussian random potential using the Feynman path-integral method.[2] The technique used in the calculation is taken from the Feynman theory of polarons.[3] It was shown that for the Gaussian impurity potentials, in three dimensions, the density of states deep in the tail goes roughly as $e^{-B(E)}$ where $B(E)$, a function of the energy, is proportional to E^n with n varying from $\frac{1}{2}$ for small autocorrelation length to 2 for large autocorrelation length. This result is in agreement with the numerical calculation by Halperin and Lax[4] and also agrees qualitatively with experiment. Such a result was also obtained by Saito and Edwards.[5] However, both of these calculations[1,5] dealt only with the exponent $B(E)$ of the density of states.

The purpose of this paper is to show that the method presented in Ref. 1 can be used to obtained the density of states deep in the tail in the form proposed by Halperin and Lax[4]:

$$\rho(E) = [A(E)/\xi^2]\exp[-B(E)/2\xi], \tag{1.1}$$

where ξ is a parameter proportional to the density of impurities and to the square of the strength of the impurity potential. In particular, we show that the prefactor $A(E)$ and the important exponent $B(E)$ can be expressed analytically in terms of well-known functions. For a Gaussian impurity potential, in three dimensions, we find $A(E) = (E_L/L)^3 a(\nu)$ and $B(E) = E_L^2 b(\nu)$ where $E_L = \hbar^2/2mL^2$ with L denoting the autocorrelation length and $\nu = (E_0 - E)/E_L$ is the energy below the mean potential in units of E_L. The two dimensionless functions $a(\nu)$ and $b(\nu)$ can be expressed analytically in terms of simple algebraic functions. For a screened charged impurity potential we obtain $A(E) = (E_Q Q)^3 a(\nu)$ and $B(E) = E_Q^2 b(\nu)$, where $E_Q = \hbar^2 Q^2/2m$ with Q being the inverse screening length, $\nu = (E_0 - E)/E_Q$ is the energy below the mean potential E_0 in units of E_Q, and $a(\nu)$ and $b(\nu)$ are two dimensionless functions which can be expressed analytically in terms of parabolic cylinder functions.

The outline of the present paper is as follows: In Sec. II we derive the density-of-states expression (1.1) for the cases of Gaussian impurity potential and screened Coulomb potential, respectively. Numerical results and graphic representations of $a(\nu)$ and $b(\nu)$ are presented in Sec. III. Discussions and a detailed comparison with the Halperin and Lax results are presented in Sec. IV.

II. DENSITY OF STATES

Following the method given in Ref. 1, we consider an electron moving among a set of N rigid impurities or scatterers, confined within a volume V, and having a density $\bar{N} = N/V$. Such a system is described by the Hamiltonian

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \sum_i v(\vec{X} - \vec{R}_i), \tag{2.1}$$

where $v(\vec{X}-\vec{R}_i)$ represents the potential of a single impurity at position $\vec{R}_i$. After averaging over all impurity configurations and assuming that the impurity potential v is weak but that their density $\bar{N}$ is high so that $\bar{N}v^2$ is finite we find that the average propagator can be expressed in the form

$$G(\vec{X}_2,\vec{X}_1;t)=\int \mathfrak{D}(\vec{X}(\tau))e^{(i/\hbar)S}\,, \tag{2.2}$$

where $\mathfrak{D}(\vec{X}(\tau))$ denotes the path integral with boundary conditions $\vec{X}(0)=\vec{X}_1$ and $\vec{X}(t)=\vec{X}_2$, and S, the action of the random system, is given as

$$S=\int_0^t d\tau\frac{m}{2}\dot{\vec{X}}^2(\tau)-\int_0^t d\tau E_0+\frac{i}{2\hbar}\bar{N}\eta^2 \times\int_0^t\int_0^t d\tau\, d\sigma\, W(\vec{X}(\tau)-\vec{X}(\sigma)). \tag{2.3}$$

Here we have taken the mean potential to be E_0 and define the autocorrelation function by

$$W(\vec{X}(\tau)-\vec{X}(\sigma))=\int d\vec{R}\,v(\vec{X}(\tau)-\vec{R})\,v(\vec{X}(\sigma)-\vec{R}). \tag{2.4}$$

The quantity η in Eq. (2.3) is a parameter which we have introduced in order to discuss more easily the behavior of the density of states as a function of the strength of the impurity potential. For an impurity potential having the Gaussian form $v(\vec{X}(\tau)-\vec{R})=u(\pi l^2)^{-3/2}\exp[-|\vec{X}(\tau)-\vec{R}|^2/l^2|$ the autocorrelation function can be written

$$W(\vec{X}(\tau)-\vec{X}(\sigma)) =u^2(\pi L^2)^{-3/2}\exp[-|\vec{X}(\tau)-\vec{X}(\sigma)|^2/L^2]\,, \tag{2.5}$$

where $L=2l$ denotes the autocorrelation length and u is another parameter introduced in order to take care of the dimension of the system. Substituting this expression into Eq. (2.3) we can write

$$S=\int_0^t d\tau\frac{m}{2}\dot{\vec{X}}^2(\tau)-\int_0^t d\tau E_0 +\frac{i}{2\hbar}\xi_L\int_0^t\int_0^t d\tau\, d\sigma\exp[-|\vec{X}(z)-\vec{X}(\sigma)|^2/L^2]\,, \tag{2.6}$$

where $\xi_L=\bar{N}\eta^2u^2/(\pi L^2)^{3/2}$ has the dimension of the energy square. The physical interpretation of this quantity was given by Saito and Edwards.[5] For an impurity potential of the screened Coulomb form

$$\eta v(\vec{X}(\tau)-\vec{R})=-Ze^2\exp[-Q|\vec{X}(\tau)-\vec{R}|]/\epsilon_0|\vec{X}(\tau)-\vec{R}|$$

we can write

$$W(\vec{X}(\tau)-\vec{X}(\sigma))=(2\pi e^4Z^2/Q\epsilon_0^2)\exp[-Q|\vec{X}(\tau)-\vec{X}(\sigma)|]\,, \tag{2.7}$$

where $\eta=e^2$ with e denoting the electronic charge, ϵ_0 the electronic dielectric constant of the pure semiconductor, Ze the charge of the impurity, and Q is the inverse screening length. The action associated with the above autocorrelation function is

$$S=\int_0^t d\tau\frac{m}{2}\dot{\vec{X}}^2(\tau)-\int_0^t d\tau E_0 +\frac{i}{2\hbar}\xi_Q\int_0^t\int_0^t d\tau\, d\sigma\exp[-Q|\vec{X}(\tau)-\vec{X}(\sigma)|]\,, \tag{2.8}$$

where $\xi_Q=2\pi Z^2e^4\bar{N}/Q\epsilon_0^2$ has the dimension of the energy square. The density of states per unit volume is then related to the diagonal part of the average propagator by

$$\rho(E)=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}dt\, G(0,0;t)\exp[(i/\hbar)Et]\,. \tag{2.9}$$

To obtain the density-of-states expression we have to find an approximate expression for G. To do this we follow the procedure given in Ref. 1 by introducing a nonlocal harmonic trial action

$$S_0=\int_0^t d\tau\left[\frac{m}{2}\dot{\vec{X}}^2(\tau)-\frac{\omega^2}{2t}\int_0^t d\sigma|\vec{X}(\tau)-\vec{X}(\sigma)|^2\right], \tag{2.10}$$

where ω is an unknown parameter to be determined. Such a translationally invariant action proves to be important for obtaining the correct behavior of the prefactor $A(E)$ in expression (1.1). By rewriting Eq. (2.2) as

$$G(0,0;t)=G_0(0,0;t)\langle\exp[(i/\hbar)(S-S_0)]\rangle_{S_0} \tag{2.11}$$

and approximating Eq. (2.11) by keeping only the first cumulant we get

$$G_1(0,0;t)=G_0(0,0;t)\exp[(i/\hbar)\langle S-S_0\rangle_{S_0}]\,, \tag{2.12}$$

where the symbol $\langle\ \rangle_{S_0}$ denotes the average with respect to the trial action S_0. From Ref. 1 the diagonal part of the zeroth-order propagator $G_0(0,0;t)$ can be calculated exactly, obtaining

$$G_0(0,0;t)=\left(\frac{m}{2\pi i\hbar t}\right)^{3/2}\left(\frac{\omega t}{2\sin(\frac{1}{2}\omega t)}\right)^3. \tag{2.13}$$

This expression differs from the free-particle one by the second factor $[\omega t/2\sin(\frac{1}{2}\omega t)]^3$ and is proved to give the correct behavior for the prefactor $A(E)$. We note that earlier unsuccessful derivations of the above expression were made by Bezak.[6] Correct derivations of this result were also obtained independently by other workers.[7,8]

From Ref. 1 the average $\langle S-S_0\rangle_{S_0}$ for the case of a Gaussian potential is given by

$$\langle S-S_0\rangle_{S_0}=-E_0t+\frac{i}{2\hbar}\xi_L\left(\frac{L^2}{4}\right)^{3/2}t\times\int_0^t dx[j_L(x)]^{-3/2}-\frac{3}{2}i\hbar\left(\frac{\omega t}{2}\cot\frac{\omega t}{2}-1\right), \tag{2.14}$$

where

$$j_L(x)=\left[\frac{L^2}{4}+\frac{i\hbar}{m\omega}\left(\sin\frac{\omega x}{2}\sin\frac{\omega(t-x)}{2}\Big/\sin\frac{\omega t}{2}\right)\right]. \tag{2.15}$$

For the case of a screened Coulomb potential after writing W in terms of Fourier components we have

$$\langle S-S_0\rangle_{S_0}=-E_0t+\frac{i}{2\hbar}\,\xi_Q\frac{Qt}{2\pi}\int_0^t dx\int\frac{d\vec{k}}{(2\pi)^3}\left(\frac{4\pi}{\vec{k}^2+Q^2}\right)^2\exp\left[-\frac{\vec{k}^2}{2}\frac{i\hbar}{m\omega}\left(\sin\frac{\omega x}{2}\sin\frac{\omega(t-x)}{2}\Big/\sin\frac{\omega t}{2}\right)\right]-\frac{3}{2}i\hbar\left(\frac{\omega t}{2}\cot\frac{\omega t}{2}-1\right). \tag{2.16}$$

Inserting the identity

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

into Eq. (2.16) and performing the $\vec{k}$ integration, we get

$$\langle S-S_0\rangle_{S_0}=-E_0t+\frac{i}{2\hbar}\xi_Q\frac{Qt}{\sqrt{\pi}}\times\int_0^t dx\int_0^\infty dy\,y\exp(-Q^2y)[j_y(x)]^{-3/2}, \tag{2.17}$$

where

$$j_y(x)=\left[y+\frac{i\hbar}{m\omega}\left(\sin\frac{\omega x}{2}\sin\frac{\omega(t-x)}{2}\Big/\sin\frac{\omega t}{2}\right)\right]. \tag{2.18}$$

Equations (2.9) and (2.13) together with Eqs. (2.14) and (2.16) represent approximate density-of-states expressions for the Gaussian potential and screened Coulomb potential, respectively.

To consider the ground-state contribution to the density of states we let $t\to\infty$. Then the density of states becomes

$$\rho_1(E)=\begin{cases}\dfrac{1}{2\pi\hbar}\displaystyle\int_{-\infty}^\infty dt\left(\frac{m}{2\pi i\hbar t}\right)^{3/2}(i\omega t)^3\exp\left[-\frac{3}{4}i\omega t-\frac{i}{\hbar}(E_0-E)t-\frac{\xi_L}{2\hbar^2}t^2\left(1+\frac{4\hbar}{2m\omega L^2}\right)^{-3/2}\right] & \text{(Gaussian potential)} \quad (2.19\text{a})\\[2ex] \dfrac{1}{2\pi\hbar}\displaystyle\int_{-\infty}^\infty dt\left(\frac{m}{2\pi i\hbar t}\right)^{3/2}(i\omega t)^3\exp\left[-\frac{3}{4}i\omega t-\frac{i}{\hbar}(E_0-E)t-\frac{\xi_QQt^2}{2\hbar^2\sqrt{\pi}}\int_0^\infty dy\,y\exp(-Q^2y)(y+\hbar/2m\omega)^{-3/2}\right] & \text{(screened Coulomb potential)}. \quad (2.19\text{b})\end{cases}$$

Using the formula[9]

$$\int_{-\infty}^\infty dt\,(it)^p\exp(-\beta^2t^2-iqt)=2^{-p/2}\sqrt{\pi}\,\beta^{-p-1}\exp(-q^2/8\beta^2)D_p(q/\beta\sqrt{2}), \tag{2.20}$$

we obtain

$$\rho_1(E)=\tfrac{1}{4}(2^{1/2}/\pi)^{1/2}\omega^3(m/2\pi\hbar)^{+3/2}\times\beta^{-5/2}\exp(-q^2/8\beta^2)D_{3/2}(q/\beta\sqrt{2}), \tag{2.21}$$

where $q=(\frac{3}{4}E_\omega+E_0-E)/\hbar$, $E_\omega=\hbar\omega$, and $D_p(z)$ denotes the parabolic-cylinder function. For a Gaussian potential,

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

and for a screened Coulomb potential,

$$\beta^2=(\xi_QQ/2\hbar^2\sqrt{\pi})\int_0^\infty dy\,y\exp(-Q^2y)(y+\hbar/2m\omega)^{-3/2}=\xi_Q\frac{\sqrt{2}}{\hbar^2}\frac{\exp}{\sqrt{\pi}}\left(\frac{1}{2}\frac{E_Q}{E_\omega}\right)D_{-3}\left(\frac{2E_Q}{E_\omega}\right)^{1/2},$$

$$E_Q=\hbar^2Q^2/2m.$$

Having obtained the above density-of-states expressions, we now consider the density of states deep in the tail. As pointed out by Halperin and Lax,[4] one can reach the low-energy tail in two equivalent ways, by letting $E\to-\infty$ ($q\to+\infty$) or keeping E constant and reducing the magnitude of the potential fluctuation by letting $\xi\to0$. Using the asymptotic properties of the parabolic-cylinder function, $D_p(z)_{z\to\infty}\exp(-\frac{1}{4}z^2)z^p$ we obtain, for the Gaussian potential,

$$\rho_1(E)=[(E_L/L)^3/\xi_L^2]a(\nu,x)\exp[-E_L^2b(\nu,x)/2\xi_L], \tag{2.22}$$

where

$$a(\nu,x)=(\tfrac{3}{4}x+\nu)^{3/2}(4+x)^3/8\sqrt{2}\,\pi^2 \tag{2.23}$$

and

$$b(\nu,x)=(\tfrac{3}{4}x+\nu)^2(1+4/x)^{3/2}, \tag{2.24}$$

with $x=E_\omega/E_L$ and $\nu=(E_0-E)/E_L$. Similarly for the screened Coulomb potential,

$$\rho_1(E)=[(E_QQ)^3/\xi_Q^2]a(\nu,z)\exp[-E_Q^2b(\nu,z)/2\xi_Q], \tag{2.25}$$

where

$$a(\nu,z)=(\tfrac{3}{2}z^{-2}+\nu)^{3/2}/8\pi\sqrt{2}\,z^6\exp(\tfrac{1}{2}z^2)D_{-3}^2(z) \tag{2.26}$$

and

$$b(\nu,z)=\sqrt{\pi}(\tfrac{3}{2}z^{-2}+\nu)^2/2\sqrt{2}\,\exp(\tfrac{1}{4}z^2)D_{-3}(z), \tag{2.27}$$

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

The parameter ω introduced in the trial action S_0 has not yet been determined. Following Halperin and Lax[4] we shall choose x or z so as to maximize $\rho_1(E)$. The justification of this procedure was given by Lloyd and Best[10] based on the variational principle. From Eq. (2.22) or (2.25), it is clear that when $\xi\to 0$, the exponential factor will become very sensitive to the choice of x or z while other factors are much more slowly varying. Hence the best choice of x or z is that which maximizes the exponential factor of Eq. (2.22) or (2.25). For the Gaussian potential the best choice of x is found to satisfy the equation

$$x^2+x-4\nu=0. \tag{2.28}$$

Since x is the ratio of the energy associated with the harmonic oscillator and the energy of the fluctuation, it must be positive. Thus keeping only the positive root, $x=\frac{1}{2}[(1+16\nu)^{1/2}-1]$, of the above equation and substituting into Eqs. (2.23) and (2.24), we obtain

$$a(\nu)=[(1+16\nu)^{1/2}-1]^{3/2}[(1+16\nu)^{1/2}+7]^{9/2}/2^{12}2^{1/2}\pi^2 \tag{2.29}$$

and

$$b(\nu)=[(1+16\nu)^{1/2}-1]^{1/2}[1+16\nu)^{1/2}+7]^{7/2}/2^8. \tag{2.30}$$

For a screened Coulomb potential the following equation is obtained:

$$D_{-3}(z)=\tfrac{1}{2}z^3(\tfrac{3}{2}z^{-2}+\nu)D_{-4}(z). \tag{2.31}$$

The complete determination of Eqs. (2.26) and (2.27) requires the solution of Eq. (2.31). Equation (2.28) or (2.31) may be compared with the Hartree-type eigenvalue equation given by Halperin and Lax.[4]

III. NUMERICAL RESULTS

Before considering the numerical evaluation of $a(\nu)$ and $b(\nu)$ let us first consider the limiting values of these functions. For the case of a Gaussian potential, it is not difficult to see that when $\nu\ll 1$, $a(\nu)=32\sqrt{2}\,\nu^{3/2}/\pi^2$ and $b(\nu)=16\nu^{1/2}$, and when $\nu\gg 1$, $a(\nu)=\sqrt{2}\,\nu^3/\pi^2$ and $b(\nu)=\nu^2$. The limiting values for the case of a screened Coulomb potential can also be evaluated analytically. For strong screening $\nu\ll 1(Q\to\infty$, or $z\to\infty)$ Eq. (2.31) has a solution $z=(2\nu)^{-1/2}$ and consequently we obtain $a(\nu)=\nu^{3/2}/\sqrt{2}\,\pi$ and $b(\nu)=2\sqrt{\pi}\,\nu^{1/2}$. For a weak screening $\nu\gg 1(Q\to 0$ or $z\to 0)$ we obtain the solution $z=[3(\pi/2)^{1/2}]^{1/3}\nu^{-1/3}$ with the condition $z^{-2}\ll\nu$. In obtaining this solution the following limiting values of the parabolic-cylinder functions $D_{-3}(z)_{z\to 0}\,\frac{1}{2}\sqrt{\frac{1}{2}\pi}$ and $D_{-4}(z)_{z\to 0}\,\frac{1}{3}$ have been used. Such a solution gives $a(\nu)=2^{1/2}/(9\pi^3)\nu^{7/2}$ and $b(\nu)=\nu^2$. For intermediate values of ν we have to solve the transcendental equation (2.31).

Besides the two dimensionless functions $a(\nu)$ and $b(\nu)$ other quantities of interest are the logarithmic derivative of the exponent $b(\nu)$, i.e., $n(\nu)=d\ln b(\nu)/d\ln\nu$ and the kinetic energy of localization $T(\nu)$. Both these quantities can also be obtained analytically as follows: for the Gaussian potential

$$n(\nu)=32\nu/[(1+16\nu)^{1/2}-1][(1+16\nu)^{1/2}+7], \tag{3.1}$$

$$T(\nu)=\tfrac{3}{4}x=\tfrac{3}{8}(\sqrt{1+16\nu}-1), \tag{3.2}$$

while for the screened Coulomb potential

$$n(\nu)=2\nu/(\tfrac{3}{2}z^{-2}+\nu), \tag{3.3}$$

$$T(\nu)=\tfrac{3}{2}z^{-2}, \tag{3.4}$$

where z is the solution of Eq. (2.31). It is easy to see that in both cases when $\nu\ll 1$, $n(\nu)\to\frac{1}{2}$, $T(\nu)/\nu\to 3$ and when $\nu\gg 1$, $n(\nu)\to 2$, $T(\nu)/\nu\to 0$.

For intermediate values of ν, we have computed the dimensionless functions $a(\nu)$, $b(\nu)$, $n(\nu)$, and $T(\nu)$ with ν varying over many orders of magnitude from $\nu=10^{-4}$ to $\nu=10^4$ for the Gaussian potential and from $\nu=10^{-3}$ to $\nu=10^3$ for the screened Coulomb potential. The results are presented in Tables I and II, respectively. For the case of a screened Coulomb potential we have used the numerical Tables of parabolic-cylinder function given in Ref. 11. The numerical results of Tables I and II are then plotted on a log-log scale for the functions $a(\nu)$ and $b(\nu)$ in Fig. 1 and on a semilog scale for $n(\nu)$ and $T(\nu)/\nu$ in Figs. 2 and 3, respectively.

TABLE I. Numerical results of the functions $a(\nu)$, $b(\nu)$, $n(\nu)$, and $T(\nu)$ for the Gaussian potential.

ν	$a(\nu)$	$b(\nu)$	$n(\nu)$	$T(\nu)$
10^4	7.717×10^{10}	1.061×10^{8}	1.971	1.496×10^{2}
$\frac{1}{2}10^4$	9.944×10^{9}	2.719×10^{7}	1.959	1.057×10^{2}
10^3	9.023×10^{7}	1.203×10^{6}	1.910	4.706×10^{1}
$\frac{1}{2}10^3$	1.236×10^{7}	3.237×10^{5}	1.876	3.317×10^{1}
10^2	1.428×10^{5}	1.738×10^{4}	1.745	1.463×10^{1}
$\frac{1}{2}10^2$	2.303×10^{4}	5.335×10^{3}	1.660	1.024×10^{1}
10^1	4.660×10^{2}	4.523×10^{2}	1.391	4.383
$\frac{1}{2}10^1$	1.038×10^{2}	1.810×10^{2}	1.250	3.000
10^0	4.929	3.168×10^{1}	0.9212	1.171
$\frac{1}{2}10^0$	1.564	1.747×10^{1}	0.8000	7.500×10^{-1}
10^{-1}	1.354×10^{-1}	5.731	0.6067	2.297×10^{-1}
$\frac{1}{2}10^{-1}$	4.884×10^{-2}	3.828	0.5614	1.281×10^{-1}
10^{-2}	4.523×10^{-3}	1.624	0.5143	2.889×10^{-1}
$\frac{1}{2}10^{-2}$	1.610×10^{-3}	1.140	0.5073	1.471×10^{-2}
10^{-3}	1.448×10^{-4}	5.067×10^{-1}	0.5015	2.988×10^{-3}
$\frac{1}{2}10^{-3}$	5.123×10^{-5}	3.580×10^{-1}	0.5007	1.497×10^{-3}
10^{-4}	4.585×10^{-6}	1.600×10^{-1}	0.5002	2.999×10^{-4}

From Fig. 1 it is easy to see that in both cases the slopes of the important exponent $b(\nu)$ vary smoothly from $\frac{1}{2}$ for $\nu \ll 1$ to 2 for $\nu \gg 1$. Such a smooth varying behavior of $b(\nu)$ is more evident in Fig. 2 and clearly indicates that the $n=\frac{1}{2}$ is characteristic of a short-range potential while the $n=2$ is characteristic of a long-range potential. From Figs. 1 and 2 it is interesting to note the similarity between the two systems for the curves $a(\nu)$ and $b(\nu)$. In Fig. 3 the kinetic energy of localization in both systems becomes very large for $\nu \ll 1$ because of the short-range nature of the potentials. This behavior becomes unimportant for $\nu \gg 1$.

IV. DISCUSSIONS AND COMPARISONS

We have applied the method developed in our previous paper to calculate the density of states for an electron moving in a Gaussian random potential using the Feynman path-integral method. Two different impurity potentials are considered: the Gaussian potential and the screened Coulomb potential. We find that the density of states deep in the tail in the first cumulant approximation (in three dimensions) can be expressed analytically as follows: for a Gaussian potential we obtain

$$\rho_1(E)=[(E_L/L)^3/\xi_L^2]a(\nu)\exp[-E_L^2 b(\nu)/2\xi_L],$$

where

$$a(\nu)=[(1+16\nu)^{1/2}-1]^{3/2}[(1+16\nu)^{1/2}+7]^{9/2}/2^{12}2^{1/2}\pi^2, \tag{2.29}$$

$$b(\nu)=[(1+16\nu)^{1/2}-1]^{1/2}[(1+16\nu)^{1/2}+7]^{7/2}/2^8, \tag{2.30}$$

and for a screened Coulomb potential

$$\rho_1(E)=[(E_Q Q)^3/\xi_Q^2]a(\nu,z)\exp[-E_Q^2 b(\nu,z)/2\xi_Q], \tag{2.25}$$

where

$$a(\nu,z)=(3/2z^2+\nu)^{3/2}/8\pi\, 2^{1/2}z^6\exp(z^2/2)D_{-3}^2(z)\ , \tag{2.26}$$

TABLE II. Numerical results of the functions $a(\nu)$, $b(\nu)$, $n(\nu)$, and $T(\nu)$ for the screened Coulomb potential. The values within the parentheses are those of Halperin and Lax (Ref. 4).

ν	z	$a(\nu)$	$b(\nu)$	$n(\nu)$	$T(\nu)$
10^3	0.1546	2.9455×10^{8} (3.098×10^{8})	1.4377×10^{6} (1.444×10^{6})	1.882	6.2758×10^{1} (6.560×10^{1})
10^2	0.3308	1.8164×10^{5} (1.888×10^{5})	2.1402×10^{4} (2.150×10^{4})	1.759	1.3807×10^{1} (1.400×10^{1})
10^1	0.7059	2.0977×10^{2} (2.197×10^{2})	4.7029×10^{2} (4.716×10^{2})	1.537	3.0103 (3.03)
10^0	1.5009	6.8155×10^{-1} (7.259×10^{-1})	1.973×10^{1} (1.956×10^{1})	1.201	6.6587×10^{-1} (6.59×10^{-1})
10^{-1}	3.2598	7.7325×10^{-3} (8.906×10^{-3})	1.9232 (1.846)	0.829	1.4116×10^{-1} (1.358×10^{-1})
10^{-2}	7.8762	2.1303×10^{-4} (2.834×10^{-4})	3.9155×10^{-1} (3.43×10^{-1})	0.585	2.4180×10^{-2} (2.316×10^{-2})
10^{-3}	22.7021	7.0405×10^{-6} (• • •)	1.1342×10^{-1} (• • •)	0.511	2.9104×10^{-3} (• • •)

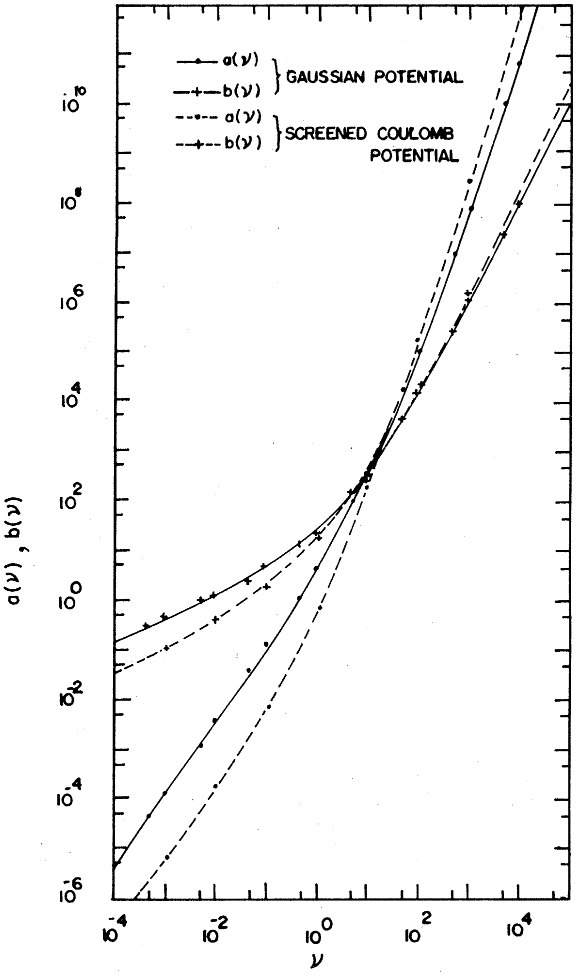

FIG. 1. Plot of prefactor $a(\nu)$ and exponent $b(\nu)$ in the density of states vs dimensionless energy ν for a Gaussian potential and a screened Coulomb potential.

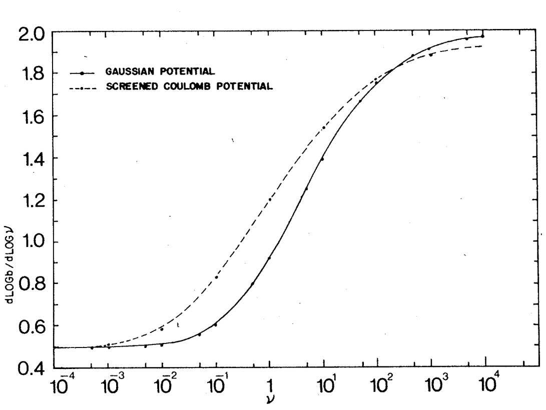

FIG. 2. Plot of logarithmic derivative $n(\nu) = d\ln b(\nu)/d\ln\nu$ of the exponent $b(\nu)$ vs the dimensionless energy ν for a Gaussian potential and a screened Coulomb potential.

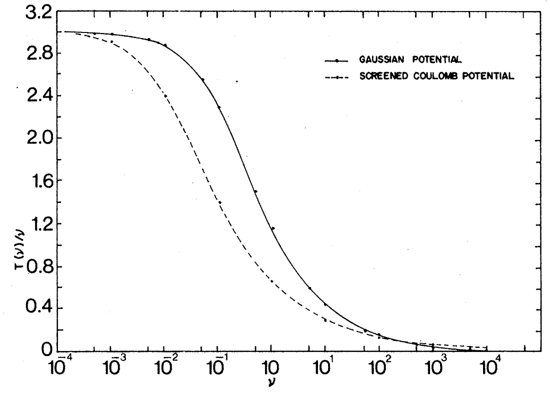

FIG. 3. Plot of the ratio of the kinetic energy to the binding energy T/ν vs the dimensionless energy ν for a Gaussian potential and a screened Coulomb potential.

$$b(\nu, z) = \pi^{1/2}(3/2z^2+\nu)^2/2^{3/2}\exp(z^2/4)\,D_{-3}(z) , \tag{2.27}$$

with z satisfying the equation

$$D_{-3}(z) = \tfrac{1}{2}z^3(3/2z^2+\nu)D_{-4}(z) . \tag{2.31}$$

The similarity in form between expressions (2.22) and (2.25) indicates that L, the autocorrelation length of the Gaussian potential, plays the role of $1/Q$ in the screened Coulomb potential.

We have also calculcated two other dimensionless functions: $n(\nu)$, the logarithmic derivative of the of the exponent $b(\nu)$, and $T(\nu)$, the kinetic energy of the localization. The results are expressed analytically as follows: for a Gaussian potential we obtain

$$n(\nu) = 32\nu/[(1+16\nu)^{1/2}-1][(1+16\nu)^{1/2}+7] , \tag{3.1}$$

$$T(\nu) = \tfrac{3}{8}[(1+16\nu)^{1/2}-1] , \tag{3.2}$$

and for a screened Coulomb potential

$$n(\nu) = 2\nu/(3/2z^2+\nu) , \tag{3.3}$$

$$T(\nu) = 3/2z^2 . \tag{3.4}$$

Numerical results as well as limiting values of these functions are given.

The above result was first obtained by Halperin and Lax[4] using the minimum-counting method. The result was obtained under the approximation that all the eigenstates at 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 was then calculated by counting the number of wells having a particular ground-state energy. The best ground-state wave function $f(\vec{x})$ was obtained by maximizing the density of states. This procedure leads to an equation

TABLE III. Comparison between the limiting values of $a(\nu)$, $b(\nu)$, $n(\nu)$, and $T(\nu)$ calculated from the present method and the method of Halperin and Lax for the case of a screened Coulomb potential. The values within the paretheses are those of Halperin and Lax (Ref. 4).

	$\nu<<1$		$\nu>>1$	
$a(\nu)$	$\simeq(1/\sqrt{2}\,\pi)\nu^{3/2}\simeq 0.23\nu^{3/2}$	$(\simeq 0.4\nu^{3/2})$	$\simeq(\sqrt{2}/9\pi^3)\nu^{7/2}\simeq 0.5\times 10^{-2}\nu^{7/2}$	$(\simeq 10^{-2}\nu^{7/2})$
$b(\nu)$	$\simeq 2\sqrt{\pi}\,\nu^{1/2}\simeq 3.54\nu^{1/2}$	$(\simeq 3\nu^{1/2})$	$\simeq\nu^2$	$(\simeq\nu^2)$
$n(\nu)$	$\simeq\frac{1}{2}$	$(\simeq\frac{1}{2})$	$\simeq 2$	$(\simeq 2)$
$T(\nu)/\nu$	$\simeq 3$	$(\simeq 3)$	$\simeq 0$	$(\simeq 0)$

$$T(\vec{x})f(\vec{x})-\mu f(\vec{x})\int[f(\vec{x}')]^2 W(\vec{x}-\vec{x}')\,d\vec{x}'=Ef(\vec{x}), \tag{4.1}$$

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. This equation may be compared with Eqs. (2.28) and (2.31) in the present approach. Using the technique developed by Hartree for solving the self-consistent equation, Halperin and Lax have calculcated the above equation numerically. The results are presented in the forms of numerical functions for $a(\nu)$, $b(\nu)$, $n(\nu)$, and $T(\nu)$.

For comparison we reproduce some of their results in Table II. Using these numerical results and the fact that the wave function associated with each minimum is small compared to the mean separation between minima, Halperin and Lax deduced that the limiting values for $a(\nu)$, $b(\nu)$, $n(\nu)$, and $T(\nu)$ must have the values given in Table III. It is interesting to note that the present method and the method of Halperin and Lax predict identical values for $n(\nu)$ and $T(\nu)/\nu$ but slightly different values for $a(\nu)$ and $b(\nu)$.

For the Gaussian potential no such comparison can be made because no result calculcated from the minimum counting method is available. However, for one-dimensional Gaussian "white noise" potential, Halperin and Lax have applied the minimum-counting method and obtained an analytical expression for the density of states deep in the tail. They have compared their result with the exact solution of Halperin.[12] We can also derive such a result using the path-integral method. Following the procedure discussed in Sec. II we readily obtain the approximate density of states in the one-dimensional Gaussian potential

$$\begin{aligned}\rho_1(E)=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}dt\left(\frac{m}{2\pi\hbar t}\right)^{1/2}\left(\frac{\omega t}{2\sin(\frac{1}{2}\omega t)}\right)\\ \times\exp\left[-\frac{1}{2\hbar^{2}}\xi\left(\frac{1}{4\pi}\right)^{1/2}t\int_0^t dx\left(\frac{L^2}{4}+\frac{i\hbar}{m\omega}\times\frac{\sin(\frac{1}{2}\omega x)\sin[\frac{1}{2}\omega(t-x)]}{\sin(\omega t/2)}\right)^{-1/2}\right.\\ \left.+\frac{1}{2}\left(\frac{\omega t}{2}\cot\frac{\omega t}{2}-1\right)+\frac{i}{\hbar}Et\right],\end{aligned} \tag{4.2}$$

where for simplicity we have set $E_0=0$ and redefined $\xi=\bar{N}\eta^2u^2$. The redefinition of ξ is necessary in the present case so as to avoid the divergency in taking the "white noise" limit. Let us now consider the ground-state contribution to the density of states. Taking the "white noise" limit $L\rightarrow 0$ expression (4.2) becomes

$$\begin{aligned}\rho_1(E)=\frac{1}{2\pi\hbar}\left(\frac{m}{2\pi\hbar}\right)^{1/2}\omega 2^{1/2}\pi^{1/2}\beta^{-3/2}\\ \times\exp(-q^2/8\beta^2)D_{1/2}(q/\beta\sqrt{2}),\end{aligned} \tag{4.3}$$

where $q=(\frac{1}{2}E_\omega-E)/\hbar$ and $\beta^2=\xi(m/2\pi\hbar)^{1/2}\omega^{1/2}2\hbar^2$. Going into the tail region $q\rightarrow\infty$ or $\beta\rightarrow 0$ and maximizing the exponent of Eq. (4.3), we obtain $E_\omega=\frac{3}{4}E$. Substituting this result into expression (4.3) yields

$$\begin{aligned}\rho_1(E)=\left(\frac{(2\pi)^{1/2}}{6}\right)\left(\frac{4}{\pi}\frac{(-E)}{\xi}\right)\\ \times\exp\left[-\left(\frac{\pi}{3}\right)^{1/2}\frac{4\sqrt{2}}{3}\frac{\hbar}{\sqrt{m}}\frac{(-E)^{3/2}}{\xi}\right].\end{aligned} \tag{4.4}$$

This result may be compared with the Halperin and

Lax[4] result

$$\rho_1^{\mathrm{HL}}(E)=\frac{1}{\sqrt{5}}\left(\frac{4}{\pi}\,\frac{(-E)}{\xi}\right)\exp\left(-\frac{4}{3}\sqrt{2}\,\frac{\hbar}{\sqrt{m}}\,\frac{(-E)^{3/2}}{\xi}\right) \tag{4.5}$$

and the exact expression of Halperin[12]

$$\rho_1^{\mathrm{exact}}(E)=\left(\frac{4}{\pi}\,\frac{(-E)}{\xi}\right)\exp\left(-\tfrac{4}{3}\sqrt{2}\,\frac{\hbar}{\sqrt{m}}\,\frac{(-E)^{3/2}}{\xi}\right)\,. \tag{4.6}$$

The agreement between ρ_1, ρ_1^{HL} and the exact asymptotic form of ρ^{exact} is remarkably good. The powers of E in the exponent and in front of the exponential are correct. The numerical factor in the exponent of ρ^{HL} is exact. Our numerical factor in the exponent, however, differs from the exact value by a factor of $\sqrt{\pi/3}=1.0233$. The numerical factors in front of the exponential for ρ_1^{HL} and ρ_1 are too small by factors of $\sqrt{5}=2.236$ and $6/\sqrt{2\pi}=2.393$, respectively. The difference between the numerical factors calculcated from the Halperin and Lax theory and the present theory is quite small being 2% and 7% for the exponent and exponential, respectively.

From the above discussion of the one-dimensional Gaussian "white noise" potential, it is shown that the numerical results obtained with the present method are not as good as that obtained with the minimum-counting method. The discrepancies between the two methods are quite small, especially the numerical factor in front of the exponent. The present method has, however, several advantages over the method of Halperin and Lax, which we shall discuss below.

(i) The calculation can be performed analytically by the introduction of a nonlocal harmonic trial action S_0. The use of a harmonic trial action is equivalent to assuming that all the fluctuating potentials have the same quadratic shape. The nonlocality of the trial action means that the harmonic potential can be anywhere in space. The possibility of using simple trial functions such as the harmonic-oscillator function for simulating the ground-state wave function $f(\vec{x})$ was suggested by Halperin and Lax as an alternative procedure for solving Eq. (4.1), but no calculation was given. In this respect our procedure is similar to that of Halperin and Lax except that we formulate the problem in terms of a Feynman path integral. Since the calculation can be performed analytically, the labor involved in the present method is much less than in the method of Halperin and Lax. For example, the solution of the Hartree-type eigenvalue equation in the one-dimensional Gaussian "white noise" potential involves the consideration of a nonlinear differential equation. In the present approach such a solution involves the maximization of the exponent of Eq. (4.3) and leads to the solution $E_\omega=\frac{3}{4}E$. Another example is the screened Coulomb potential where the solution of the Hartree-type eigenvalue equation (4.1) is reduced to just solving a transcendental equation (2.31) involving two parabolic cylinder functions. As a result several limiting values of the dimensionless functions can be easily obtained, such as those given in Table III.

(ii) The calculation can be improved by going beyond the first cumulant approximation. In the second cumulant approximation, the average propagator can be expressed

$$\begin{aligned}G_2(\vec{x}_2,\vec{x}_1;t)={}&G_0(\vec{x}_2,\vec{x}_1;t)\\&\times\exp\{\langle S-S_0\rangle_{S_0}+\tfrac{1}{2}[\langle(S-S_0)^2\rangle_{S_0}\\&-\langle S-S_0\rangle_{S_0}^2]\}\,.\end{aligned} \tag{4.7}$$

It is not hard to see that the above equation involves the averages $\langle x(\tau)\rangle_{S_0}$, $\langle x(\tau)x(\sigma)\rangle_{S_0}$, and $\langle x(\tau)x(\sigma)x(\tau')x(\sigma')\rangle_{S_0}$. These averages can be obtained with the aid of the characteristic functional given in the Appendix of Ref. 1. The second cumulant approximation may be compared roughly with the second-order correction discussed by Halperin and Lax[13] where the difference between the actual random potential and the average well shape is treated as a small perturbation. Halperin and Lax[13] have shown that the effect of the second-order correction is to modify the prefactor but not the exponent $B(E)$. They find that for the one-dimensional "white-Gaussian-noise" potential the second-order correction is to bring the numerical factor in front of the exponential from $1/\sqrt{5}$ to $\exp\frac{13}{18}/\sqrt{5}$. The path-integral method also confirms their conclusion. Recently, Gross[14] has calculcated the second cumulant correction to the one-dimensional "white-Gaussian-noise" potential and has found that the way to make the correction is to change the numerical factor in front of the exponent from $\sqrt{\pi/3}$ to $\sqrt{64\pi/201}=1.000\,15$, while the numerical factor in front of the exponential becomes $\frac{4}{3}\sqrt{\pi/3}\;1/\sqrt{2}$.

(iii) The method can be used to obtain the density of states at high and intermediate energies. For high energies which correspond to allowing $t\rightarrow 0$, the density of states for the screened Coulomb potential becomes

$$\begin{aligned}\rho_1(E)={}&\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}dt\left(\frac{m}{2\pi i\hbar t}\right)^{3/2}\\&\times\exp\left(-\frac{1}{4\hbar^2}\,\zeta^2t^2+\frac{i(E-E_0)t}{\hbar}\right),\end{aligned} \tag{4.8}$$

where $\zeta=(4\pi\overline{N}/Q)^{1/2}(Ze^2/\epsilon_0)$. With the aid of Eq. (2.20), the above expression can be written

$$\rho_1(E)=\frac{m^{3/2}}{2\pi^2 2^{3/4}\hbar^3}\left(\frac{\zeta}{2}\right)^{1/2}\exp\left(\frac{-(E-E_0)^2}{2\zeta^2}\right)D_{-3/2}\left(-\frac{\sqrt{2}\,(E-E_0)}{\zeta}\right). \tag{4.9}$$

Since $t\to 0$ corresponds to $|E-E_0|\to\infty$, we obtain the asymptotic formulas

$$\rho_1(E)=\begin{cases}\dfrac{m^{3/2}}{\sqrt{2}\,\pi^2\hbar^3}\sqrt{E-E_0}\,, & \text{for } \dfrac{E-E_0}{\zeta}\gg 1\\[2ex] \dfrac{m^{3/2}}{8\pi^2\hbar^3}\zeta^{1/2}\left(\dfrac{E_0-E}{\zeta}\right)^{3/2}\exp\left[-\dfrac{(E-E_0)^2}{\zeta^2}\right], & \text{for } \dfrac{(E-E_0)}{\zeta}\ll -1\,.\end{cases} \tag{4.10}$$

The first of these expressions is the free-electron-gas result and the second is the well-known band tail result of Kane.[15] Note that for high energies the unknown parameter ω disappears from the density-of-states expression (4.9). For intermediate energies, we have to keep t finite in the density-of-states expression. Although the density of states cannot be reduced to a simple form as in cases of high and low energies, the calculation can still be performed with the aid of a computer. The real difficulty in the present case, however, is the unknown parameter ω which cannot be obtained by maximizing the density of states because, as shown by Lloyd and Best, it does not satisfy the variational principle. They showed that the correct expression to be maximized is not $\rho(E)$ or $\ln\rho(E)$ as anticipated previously by Kane,[15] Halperin and Lax,[4] and Edwards,[16] but instead the following functional:

$$P(E)=\int^{E} N(E')\,dE'\,, \tag{4.11}$$

where $N(E')$ is the integrated density of states

$$N(E)=\int^{E}\rho(E')\,dE'\,. \tag{4.12}$$

As $E\to-\infty$ this variational principle is equivalent to maximizing the density of state because $\rho(E)$ is dominated by its exponential decay. We note that the method of Halperin and Lax cannot be used directly to obtain the density of states at high and intermediate energies because they have neglected excited states in the potential well formed by the fluctuating potential. The extension of Halperin and Lax may be made by choosing the trial wave function $f(\vec{x})$ orthogonal to the previously obtained ground-state wave function.

(iv) The method can be applied to the evaluation of the density of states with general statistics including the consideration of correlations among the impurity centers.[17,18] Then the average propagator can be developed in a cumulant series. For a completely random system the following average propagator may be considered[1]:

$$G(\vec{x}_2,\vec{x}_1;t)=\int\mathfrak{D}(\vec{x}(\tau))\exp\left\{\frac{i}{\hbar}\int_0^t d\tau\,\frac{m}{2}\dot{\vec{x}}^2(\tau)+\bar{N}\int d\vec{R}\left[\exp\left(-\frac{i}{\hbar}\int_0^t d\tau\,v(\vec{x}(\tau)-\vec{R})\right)-1\right]\right\}. \tag{4.13}$$

One may proceed in the calculation as before for the Gaussian statistics. The density of states again can be expressed in terms of the prefactor $A(E)$ and the exponent $B(E)$. Shklovskii and Efros[19] have considered the exponent $B(E)$ using the generalization of the "uniform cluster" approximation of Kane.[15] The path-integral derivation of $B(E)$ using a local trial action has been worked out by Friedberg and Luttinger.[20] However, both methods cannot give the correct behavior of $A(E)$ because $A(E)$ requires the use of a translationally invariant trial action. The present method is readily applicable to this problem.

The results obtained in this paper can be applied to physical systems, for instance the screened Coulomb potential can be used to study the band-tail parameters in heavily doped semiconductors. The physical quantities to be studied in this case are the Fermi energy, the optical absorption, spontaneous and stimulated emissions etc. This study was carried out by Hwang,[21] and Casey and Stern.[22] Hwang used the numerical results of Halperin and Lax[4] interpolating with the distorted parabolic band of Bonch-Bruviech,[23] while Casey and Stern combined the Halperin and Lax result with the result of Kane.[15] We may calculate these band-tail parameters using the analytical density of states expression obtained in this paper. It is expected that a similar conclusion can be reached with much less computational effort. For a Gaussian potential the result can be used to study the noncrystalline structures such as polycrystallines and amorphous semiconductors. Since one usually does not know the detailed shape of the noncrystalline structures, the autocorrelation length can be estimated from experiment, such as from the radial distribution function. A calculation along this direction was considered by Stern.[24]

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