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Impurity-band density of states in heavily doped semiconductors: A variational calculation

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The impurity-band density of states $\rho_1(E)$ for electrons in the field of dense, random attractive impurities is calculated in the tail region using an analytic expression derived previously by one of us (V.S.). The analytic expression contains a single free parameter that fixes the curvature of the trial harmonic well which models the Gaussian random potential seen by the electrons. This parameter is determined here by implementing the rigorous variational principle derived by Lloyd and Best. The resulting density of states is significantly larger than that obtained by Halperin and Lax, although the Halperin and Lax values can be reproduced if the free parameter is determined as in their theory by minimizing the exponent in $\rho_1(E)$. The present $\rho_1(E)$ crosses the Kane value at higher E. A simple interpolation scheme is proposed to determine $\rho(E)$ for all energies E; use the present tail $\rho(E)$ from low E up to where it crosses the Kane value and thereafter use $\rho^{\text{Kane}}(E)$.

I. INTRODUCTION

A. The model

The impurity-band density of states $\rho(E)$ available to electrons in a solid containing a high concentration of randomly distributed, attractive impurity centers remains a problem of continuing importance in semiconductor technology.[1] Models of this system usually begin with electrons in a pure solid having a conduction band of energy lying above and separated from a valence band by an energy gap. The attractive centers introduce impurity states of energy E lying in the gap just below the bottom of the conduction band. At high concentration (many centers lying within the wave function of a single electron which can extend over several hundred angstroms) the impurity states themselves form a band. This band joins onto the conduction band and has a low-energy, exponential tail reaching deep into the band gap.

The most complete calculation of $\rho(E)$ in the low-energy, deep-tail region of the impurity band remains the optimal fluctuation results of Halperin and Lax.[2] Their theory is the quantum counterpart of the original semiclassical theory of Kane.[3,4] Quantum effects were included by adding the zero-point energy to the electron states (kinetic energy of localization), which raises the electron-state energies and reduces $\rho(E)$ at small E below the semiclassical value obtained by Kane. The extensive and wide-ranging work in this field has recently been exhaustively reviewed[1,5-8] and we refer the reader to these reviews for full references. Here we focus only on the density of states.

Wolff[9] and more recently Hwang[10] and Casey and Stern[11] have shown that in the presence of impurities the interelectron interaction can be incorporated into a single electron effective mass m^* plus a rigid shift of the bands, provided the electrons are regarded as moving in a screened Coulomb potential due to the impurities. Hence for parabolic bands we may model the impurity system by considering a single free electron of mass m^* in the presence of N impurities in volume Ω (density $\bar{N}=N/\Omega$). The corresponding Hamiltonian is

$$H=-\frac{\hbar^2\nabla^2}{2m^*}+\sum_{i=1}^{N} v(\vec{r}-\vec{R}_i)\,. \tag{1}$$

Here

$$v(\vec{r}-\vec{R})=-\frac{Ze^2}{\epsilon_0}\frac{e^{-Q|\vec{r}-\vec{R}|}}{|\vec{r}-\vec{R}|} \tag{2}$$

is the screened potential due to an impurity of charge Z having screening length Q^{-1} and located at point R. The ϵ_0 is the dielectric constant and the R_i are randomly distributed throughout the solid. If the correlations in the potential beyond the mean

$$\int d\vec{R}\, v(\vec{r}-\vec{R})=E_0 \tag{3}$$

and the quadratic

$$\int d\vec{R}\, v(\vec{r}-\vec{R})v(\vec{r}'-\vec{R})=W(\vec{r}-\vec{r}') \tag{4}$$

are neglected, this model is an example of a single particle moving in a Gaussian random potential[12] (higher correlations in the potential neglected). For the example of the screened Coulomb interaction (2) in (4),

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$$\bar{N}W(\vec{r}-\vec{r}') = \xi_Q e^{-Q|\vec{r}-\vec{r}'|}, \tag{5}$$

where $\xi_Q = 2\pi Z^2 e^4 \bar{N}/(Q\epsilon_0^2)$ has dimensions of energy squared and measures the magnitude of the variance or fluctuation in the random potential about the mean E_0.

B. The variational principle

In this paper we evaluate numerically the impurity band $\rho(E)$ throughout the deep-tail region for a single electron in a Gaussian random potential (5). This is done by implementing the variational principle derived by Lloyd and Best[13] which states that the optimum $\rho(E)$ should maximize the function

$$P(E) = \int_{-\infty}^{E} dE' \int_{-\infty}^{E'} dE'' \rho(E''). \tag{6}$$

For $\rho(E)$ we use the analytic expression derived earlier[14] (referred to here as I) by one of us (V.S.), which is valid in the deep tail region. This $\rho(E)$ contains one variational parameter to be determined by (6). We compare the $\rho(E)$ determined by this rigorous principle (denoted case 1) with the approximate $\rho(E)$ determined by maximizing $\rho(E)$ itself (denoted case 2) and by minimizing the exponent in the exponential portion of $\rho(E)$ (denoted case 3). We find that the $\rho(E)$ obtained by maximizing $P(E)$ and $\rho(E)$ differ little but that the $\rho(E)$ obtained by minimizing the exponent only differs substantially from the first two for random potentials having large fluctuations (large ξ_Q). Halperin and Lax[2] considered the last case only and in this case our $\rho(E)$ agrees well numerically with Halperin and Lax.

C. The density of states

In I the random potential having variance $W(\vec{r}-\vec{r}')$ seen by the electron is modeled by a single, nonlocal harmonic potential. The curvature $\frac{1}{2}\omega^2$ of the model harmonic potential is the free parameter which must be determined at each E by one of the variational principles referred to above. This procedure follows in spirit the minimum counting method of Halperin and Lax who determined at each E the single best ground-state wave function which most often represented the possible wave functions of the electrons in the random system. Abrams and Edwards[15] earlier suggested using a harmonic well. This corresponds, in the Halperin and Lax theory, to choosing Gaussian ground-state wave functions.

The full expression for $\rho(E)$ valid at all E obtained in I is lengthy and requires numerical integration. However, in the limit of low E ($E \to -\infty$) in the impurity-band-tail region, where only the ground states of the electrons need be included, $\rho(E)$ simplifies to an analytic expression. This may be written in the same form as introduced by Halperin and Lax as

$$\rho_1(E) = \frac{A(E)}{\xi_Q^2} \exp[-\tfrac{1}{2}B(E)/\xi_Q], \tag{7}$$

where

$$A(E) = (QE_Q)^3 a(\nu, z),$$
$$B(E) = E_Q^2 b(\nu, z). \tag{8}$$

Here $E_Q = \hbar^2 Q^2/2m^*$ is the energy associated with the impurity potential and all energies are expressed in units of E_Q. For example, $\nu = (E_0 - E)/E_Q$ is the electron energy measured away from the mean potential E_0 in units of E_Q and $z = (2E_Q/\hbar\omega)^{1/2}$ is a convenient reduced variational parameter, replacing ω. In the harmonic model the kinetic (zero-point) energy of electron localization is just $\frac{3}{4}\hbar\omega$ and in reduced units is $T = (\frac{3}{4})\hbar\omega/E_Q = \frac{3}{2}z^{-2}$. Finally, the analytic expressions for the "universal," dimensionless functions $a(\nu, z)$ and $b(\nu, z)$ obtained in I are

$$a(\nu, z) = (T+\nu)^{3/2} \Big/ \left[8\pi\sqrt{2}\, z^6 \exp\left(\frac{z^2}{2}\right) D_{-3}^2(z)\right], \tag{9}$$

$$b(\nu, z) = (T+\nu)^2 \sqrt{\pi} \Big/ \left[2\sqrt{2} \exp\left(\frac{z^2}{4}\right) D_{-3}(z)\right], \tag{10}$$

where $D_p(z)$ is the parabolic cylinder function.[16]

The subscript 1 on $\rho_1(E)$ means that the first-order cumulant correction for the difference between W and the harmonic model has been evaluated exactly. Higher-order cumulants which correspond approximately to the higher-order corrections considered by Halperin and Lax[17] have been ignored.

The variational equation to determine z obtained from maximizing $P(E)$ is, in reduced units,

$$\int_{\nu}^{\infty} d\nu' (\nu - \nu') a(\nu', z) e^{-b(\nu', z)/2\xi'} \times \left\{ \left[\frac{2D_{-4}(z)}{D_{-3}(z)} - \frac{1}{z}\left(\frac{T}{T+\nu'} + 2\right)\right] - \frac{b(\nu', z)}{2\xi'}\left(\frac{D_{-4}(z)}{D_{-3}(z)} - \frac{2z^{-3}}{(T+\nu')}\right)\right\} = 0. \tag{11}$$

The equation for z obtained from maximizing $\rho_1(E)$ itself corresponds to setting the term in curly brackets in (11) equal to zero, i.e.,

$$\left\{\left[\frac{2D_{-4}(z)}{D_{-3}(z)}-\frac{1}{z}\left(\frac{T}{T+\nu}+2\right)\right]-\frac{b(\nu,z)}{2\xi'}\left(\frac{D_{-4}(z)}{D_{-3}(z)}-\frac{2z^{-3}}{(T+\nu)}\right)\right\}=0. \quad (12)$$

The equation for z obtained from minimizing the exponent $B(E)$ in $\rho_1(E)$ corresponds to setting the term in the last large parentheses in (12) equal to zero, i.e.,

$$\left(\frac{D_{-4}(z)}{D_{-3}(z)}-\frac{2z^{-3}}{(T+\nu)}\right)=0. \quad (13)$$

The expression (7), plus one of the three equations (11), (12), or (13) for z, completely determines the density of states in the band-tail region. The $\rho_1(E)$ evaluated for the three methods of determining z are shown in Figs. 6–9 for values of the reduced fluctuation parameter $\xi'=\xi_Q/E_Q^2=50$, 5, 0.5, and 0.05.

In Sec. II the origin of $\rho_1(E)$ is outlined. The variational equations (11)–(13) for z are derived in Sec. III. The numerical results for z, $a(\nu,z)$, $b(\nu,z)$, and the density of states are presented in Sec. IV. A summary and conclusion are given in Sec. V. The corrections to (7) for excited-state contributions to $\rho_1(E)$ are discussed in the Appendix.

II. THE DENSITY OF STATES

The density of states per unit volume

$$\rho(E)=\frac{1}{\Omega}\sum_s \delta(E-E_s) \quad (14)$$

can be expressed in terms of the propagator for a single electron moving in the field of N impurities as

$$\rho(E)=\frac{1}{\pi\hbar}\,\mathrm{Re}\int_0^\infty dt\, e^{iEt/\hbar}\bar{G}(0,0,t), \quad (15)$$

where $\bar{G}(\vec{r}_2,\vec{r}_1,t)$ is the retarded propagator in the coordinate representation [$(i\hbar)$ times the usual retarded Green's function] averaged over all impurity positions, assumed randomly distributed. This propagator is expressed in I as a Feynman path integral[15,18-26]

$$\bar{G}(\vec{r}_2,\vec{r}_1,t)=\int D(\vec{r}(\tau))e^{(i/\hbar)S}, \quad (16)$$

where for a Gaussian random potential the action is

$$S=\int_0^t d\tau\left(\frac{m^*}{2}\dot{\vec{r}}^2(\tau)-E_0+\frac{i}{2\hbar}\bar{N}\int_0^t d\tau' W(\vec{r}(\tau)-\vec{r}(\tau'))\right). \quad (17)$$

E_0 and W are given by (3) and (4), respectively. In I the full action S in (17) is approximated by a nonlocal harmonic model or "trial" action[27]

$$S_0=\int_0^t d\tau\left(\frac{m^*}{2}\dot{\vec{r}}^2(\tau)-E_0-\frac{\omega^2}{2t}\int_0^t d\tau'\,|\vec{r}(\tau)-\vec{r}(\tau')|^2\right) \quad (18)$$

for which the diagonal part of $\bar{G}$ in (16) can be evaluated exactly. This constitutes the zero-order approximation $\bar{G}_0$ to $\bar{G}$. Equation (16) can also be rearranged in terms of G_0 and S_0 as

$$\bar{G}=\bar{G}_0\left\langle\exp\left(\frac{i}{\hbar}\right)(S-S_0)\right\rangle_0, \quad (19)$$

where $\langle\ \rangle_0$ is the average with respect to the trial action S_0. By keeping only the first-order cumulant in (19) we obtain the first-order approximation to $\bar{G}$,

$$G_1=G_0\exp\left(\frac{i}{\hbar}\langle S-S\rangle_0\right). \quad (20)$$

The diagonal part of $\bar{G}_1$ may also be evaluated exactly and, when substituted into (15), gives the density of states of

$$\rho_1(E)=\frac{1}{\pi\hbar}\,\mathrm{Re}\int_0^\infty dt\left[\left(\frac{m^*}{2\pi i\hbar t}\right)^{1/2}\left(\frac{\omega t}{2\sin(\frac{1}{2}\omega t)}\right)\right]^3 \times\exp\left[-\frac{i}{\hbar}(E_0-E)t-\frac{1}{2\hbar^2}\xi_Q\frac{Qt}{\sqrt{\pi}}\int_0^t dx\int_0^\infty dy\, y e^{-Q^2y}j(x,y)^{-3/2}+\frac{3}{2}\left(\frac{\omega t}{2}\cot\frac{\omega t}{2}-1\right)\right], \quad (21)$$

where

$$j(x,y)=\left[y+\frac{i\hbar}{m^*\omega}\left(\sin\frac{\omega x}{2}\sin\frac{\omega(t-x)}{2}\Big/\sin\frac{\omega t}{2}\right)\right].$$

In (21) the term in the square brackets is $G_0(0,0,t)$ while the exponential term is the first cumulant correction, aside from $e^{iEt/\hbar}$.

To obtain the limit of $\rho_1(E)$ valid in the tail region of the impurity band we first take the $t\to\infty$ limit of the integrand in (21). This means only the ground states,[18] the lowest-energy states, will be retained in $\rho_1(E)$. The integrals in (21) can then be evaluated exactly and, in reduced units, the result is

$$\rho_1(\nu,z)=\frac{Q^3}{E_Q\xi'^{5/4}}\frac{a(\nu,z)}{b(\nu,z)^{3/4}} \times e^{-b(\nu,z)/4\xi'}D_{3/2}\left(\left(\frac{b(\nu,z)}{\xi'}\right)^{1/2}\right). \quad (22)$$

In the limit of large $b(\nu,z)/\xi'$ the asymptotic expression for the parabolic cylinder function is

$$D_p(x)=e^{-x^2/4}x^p\left(1-\frac{p(p-1)}{2}\frac{1}{x^2}+\cdots\right). \quad (23)$$

If we neglect the term in x^{-2} in (23) we obtain Eq. (7) for $\rho_1(\nu,z)$, i.e.,

$$\rho_1(\nu,z)=\frac{Q^3}{E_Q\xi'^2}a(\nu,z)e^{-b(\nu,z)/2\xi'}. \quad (7')$$

The corrections to (7′) for the neglected terms in (23) and for excited-state contributions at higher E are discussed in Sec. IV C and the Appendix.

We may also obtain the semiclassical (SC) limit of $\rho_1(E)$ from the full $\rho_1(E)$ in (21). This is obtained by letting $t\to 0$ in the integrand of (21), which corresponds to retaining only high-electron-energy states in $\rho_1(E)$. The integrals in (21) can again be performed, giving

$$\rho_1^{SC}(E)=\frac{m^{*3/2}}{4\pi^2\hbar^3}\xi_Q^{1/4}e^{-(E-E_0)^2/4\xi_Q}D_{-3/2}\left(\frac{E_0-E}{\sqrt{\xi_Q}}\right), \quad (24)$$

which is the result derived by Kane.[3] In the limit $|E-E_0|\to\infty$ this becomes

$$\rho_1^{SC}(E)=\begin{cases}\dfrac{m^{*3/2}}{4\pi^2\hbar^3}\dfrac{\xi_Q}{(E_0-E)^{3/2}}e^{-(E-E_0)^2/2\xi_Q}, & \dfrac{E-E_0}{\sqrt{\xi_Q}}\ll -1 \quad (25a)\\ \dfrac{m^{*3/2}}{\sqrt{2}\pi^2\hbar^3}\sqrt{E-E_0}, & \dfrac{E-E_0}{\sqrt{\xi_Q}}\gg 1. \quad (25b)\end{cases}$$

Here (25a) is Kane's well known band tail $\rho_1(E)$ while (25b) is the free-electron or parabolic-band value valid for positive $E-E_0$ only. Note that (24) is independent of the variational parameter. This is because at $t\to 0$ only the free particle $\bar{G}_0$ survives in (21) and the semiclassical $\rho_1(E)$ is independent of the harmonic model action selected here. It is for this reason that (24) agrees exactly with Kane's density of states.

III. THE VARIATIONAL EQUATIONS

In this section we develop the equations (11), (12), and (13), which are needed to determine the variational parameter z based on (1) the Lloyd-Best[13] variational principle, (2) maximizing $\rho_1(E)$, and (3) minimizing the exponent $B(E)$ in $\rho_1(E)$, respectively.

A. The Lloyd-Best variational principle: Case 1

Lloyd and Best[13] showed that the density of states $\rho_1(E)$ at energy E should maximize the pressure

$$P(E,z)=\int_{-\infty}^{E}dE'\int_{-\infty}^{E'}dE''\rho(E'',z) \quad (26)$$

of a hypothetical free-fermion system. This may be used here to determine the free parameter z in a band-tail expression for $\rho(E,z)$, since values of $\rho(E'',z)$ up to energy E only are needed. To simplify (26) we do an integration by parts

$$P(E,z)=E'\int_{-\infty}^{E'}dE''\rho(E'',z)\Big|_{-\infty}^{E}-\int_{-\infty}^{E}\rho(E',z)dE' \quad (27)$$

and use $\rho(-\infty,z)=0$ to write (27) as

$$P(E,z)=\int_{-\infty}^{E}(E-E')\rho(E',z)dE'. \quad (28)$$

In terms of the reduced energy $\nu=(E_0-E)/E_Q$, this is

$$P(\nu,z)=-E_Q^2\int_{\nu}^{\infty}(\nu-\nu')\rho(\nu',z)d\nu'. \quad (29)$$

On substituting (7′) for $\rho(\nu',z)$ in (29) and maximizing $P(\nu,z)$ with respect to z $[dP(\nu,z)/dz=0]$, we obtain the variational equation (11) for z.

B. Maximizing $\rho_1(E)$: Case 2

It is more convenient to maximize $\ln\rho_1(\nu,z)$. Employing (7′) this requires

$$\frac{d\ln\rho_1(\nu,z)}{dz}=\frac{d\ln a}{dz}-\frac{1}{2\xi'}\frac{db}{dz}=0. \quad (30)$$

On differentiating the logarithm of (9) and using the recursion relation for parabolic cylinder functions,[16]

$$\frac{dD_p(z)}{dz}=-\tfrac{1}{2}zD_p(z)+pD_{p-1}(z), \quad (31)$$

the first term in (30) is

$$\frac{d\ln a(\nu,z)}{dz}=6\left(\frac{D_{-4}(z)}{D_{-3}(z)}-\frac{3}{4}\frac{z^{-3}}{(T+\nu)}-\frac{1}{z}\right). \quad (32)$$

Similarly, differentiating (10) and using (31), the second term in (30) is

$$\frac{db(\nu,z)}{dz}=3b(\nu,z)\left(\frac{D_{-4}(z)}{D_{-3}(z)}-\frac{2z^{-3}}{(T+\nu)}\right). \quad (33)$$

Substituting (32) and (33) into (30) gives the variational equation (12) to determine z in this case.

C. Minimizing the exponent $b(\nu,z)$: Case 3

The variational equation in this case is now obtained trivially by setting (33) equal to zero, which gives Eq. (13).

IV. NUMERICAL RESULTS

In this section we present numerical solutions for the reduced variational parameters $z=(2E_Q/\hbar\omega)^{1/2}$ and numerical values for the density of impurity-band states $\rho_1(E)$ for a single-spin state.

A. The variational parameter

The values of z, obtained by (1) solving (11), which corresponds to maximizing $P(E)$, (2) solving (12), which corresponds to maximizing $\rho_1(E)$, and (3) solving (13), which corresponds to minimizing the exponent $B(E)$ in $\rho_1(E)$, are shown in Fig. 1. The z values are shown as a function of the reduced energy $\nu=(E_0-E)/E_Q$ for four different values of the reduced parameter

$$\xi'=\frac{\xi_Q}{E_Q^2}=\frac{8\pi m^{*2}Z^2e^4\bar{N}}{\hbar^4\epsilon_0^2Q^5}, \tag{34}$$

which measures the magnitude of the fluctuation in the random potential.

We note first that in the most approximate case (3), z is independent of ξ'. Next, from Fig. 1 we see that in the limit $\nu\gg1$ all three cases give the same values for z. In fact, it is possible to show in the limit $\nu\gg1$ (with $\nu\gg T$) that the three equations (11), (12), and (13) for z become identical. Physically, since $E_Q=\hbar^2Q^2/2m^*$, the $\nu=(E_0-E)/E_Q$ is proportional to the square of the impurity-potential screening length Q^{-1}. Hence $\nu\gg1$ corresponds either to a long-range impurity potential or to energies $E\to-\infty$ lying in the very deep band-tail region (or both). Clearly, large ξ' also corresponds to a long-range impurity potential ($\xi'\propto Q^{-5}$). Since for large ξ' case (3) differs substantially from both (1) and (2), the three cases are only strictly identical for $E\to-\infty$. In summary, cases (1) and (2) remain essentially identical over the physically interesting range of ν ($0\leq\nu\leq20$) except for small values of the fluctuation parameter ξ'. However, case (3) gives substantially different z values except in the limit $E\to-\infty$).

To display the role of the kinetic energy of electron localization $T=\frac{3}{2}z^{-2}=\frac{3}{4}(\hbar\omega/E_Q)$, we plot $T/\nu=\frac{3}{4}\hbar\omega/(E_0-E)$ versus the reduced energy ν in Fig. 2. From this figure we see that $T/\nu\to0$ for $\nu\gg1$ in all three cases as expected. When $T/\nu\to0$ the kinetic (zero-point) energy is negligible and semiclassical theory is applicable. This limit can be reached physically only for a wide impurity potential having a long screening length Q^{-1} ($\nu\propto Q^{-2}$).

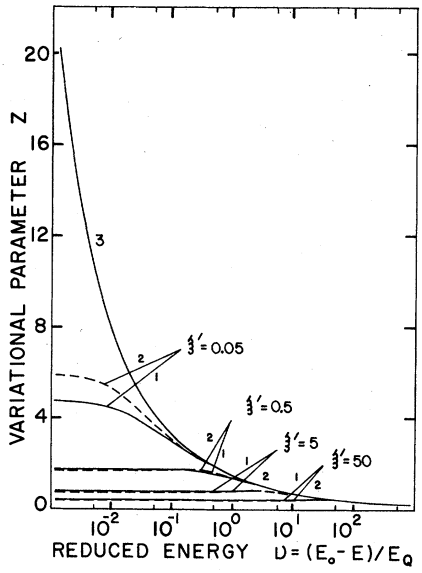

FIG. 1. Variational parameter z as a function of reduced energy $\nu=(E_0-E)/E_Q$, determined from (1) the Lloyd-Best variational principle, Eq. (11), (2) maximizing $\rho_1(E)$, Eq. (12), and (3) minimizing the exponent $b(\nu,z)$ in $\rho_1(E)$, Eq. (13). Four values of the parameter

$$\xi'=\frac{8\pi m^{*2}Z^2e^4\bar{N}}{\hbar^4Q^5\epsilon_0^2},$$

which sets the magnitude of fluctuation in the random potential, are shown. Case 3 is independent of ξ'.

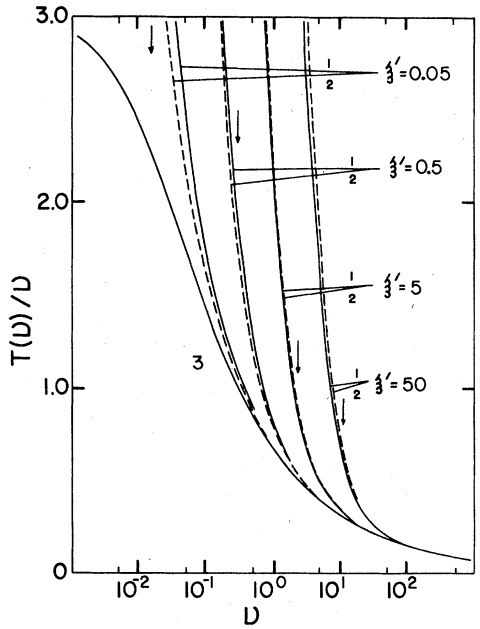

FIG. 2. Ratio of the kinetic energy of electron localization $T=\frac{3}{4}\hbar\omega/E_Q=\frac{3}{2}z^2$ to the reduced energy ν, $T(\nu)/\nu$, as a function of ν for 4 values of ξ'. The z and T are determined by the same three equations as noted in Fig. 1. $T(\nu)/\nu$ in case 3 is independent of ξ'. The arrows indicate the value of ν below which the deep-tail approximation in $\rho_1(E)$ ceases to be valid at each ξ'.

However, for $\nu \ll 1$ the kinetic energy of localization is most important and differs substantially in the three cases. When $P(E)$ and $\rho_1(E)$ are maximized, T/ν can be very large. However, if we restrict ourselves to energies in the deep-tail region, where $E_0 - E$ must remain reasonably large, the ratio T/ν will always remain finite. It is only in the approximate case of minimizing $B(E)$ considered by Halperin and Lax that T/ν approaches the special value of 3 for $\nu \ll 1$. It is not clear that there is any meaning to this special value of 3.

B. The density of states

Having obtained the reduced variational parameter z for each ν we can now calculate the universal, dimensionless functions $a(\nu, z)$ and $b(\nu, z)$ appearing in the density of states $\rho_1(E)$ in (7). The resulting $a(\nu, z)$ and $b(\nu, z)$ are plotted in Figs. 3 and 4, respectively. We note again that in case 3, $a(\nu, z)$ and $b(\nu, z)$ are independent of the fluctuation parameters ξ'. Also, the $a(\nu, z)$ and $b(\nu, z)$ differ somewhat in cases 1 and 2 but these differences tend to cancel when $a(\nu, z)$ and $b(\nu, z)$ are substituted in $\rho_1(E)$. The logarithmic exponent of $b(\nu, z)$ is displayed in Fig. 5.

To complete the calculation of the density of states we include calculations of Kane's semiclassical limit impurity-band density of states and the parabolic band value. As noted in Sec. II and in I,

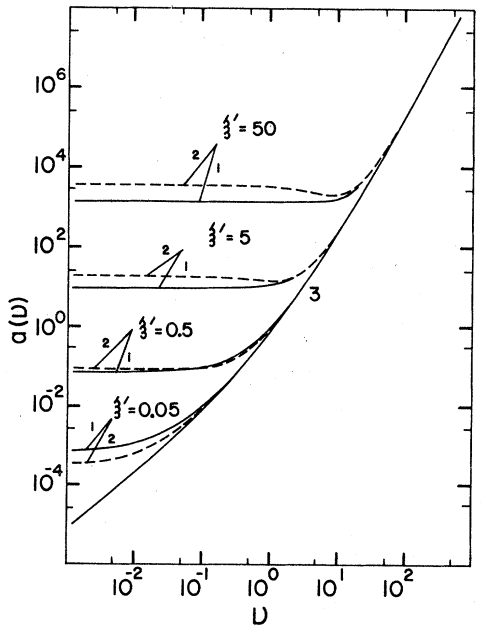

FIG. 3. Values of the dimensionless function $a(\nu, z)$ of Eq. (9) with z determined: (1) from Eq. (11), (2) from Eq. (12), and (3) from Eq. (13).

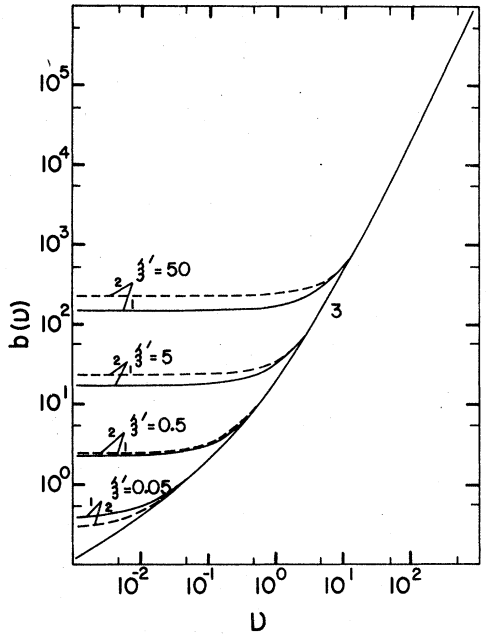

FIG. 4. Dimensionless function $b(\nu, z)$ of Eq. (10) with z determined as noted below Fig. 1.

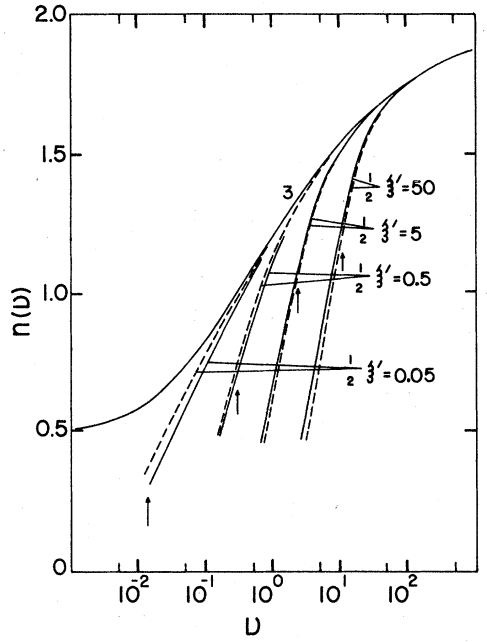

FIG. 5. Logarithmic derivative of the exponent $b(\nu)$ in $\rho_1(E)$,

$$n(\nu) = (d \log b)/(d \log \nu) = 2\nu/(T + \nu)$$

for four values of ξ' with z determined as noted below Fig. 1. Case 3 corresponds to the Halperin and Lax limit and is independent of ξ'. The arrows indicate the value of ν below which the deep-tail approximations in $\rho_1(E)$ ceases to be valid for each ξ'. In the limit $\xi' \to 0$ all three cases should reach $n = \frac{1}{2}$.

these can be obtained by retaining only the higher-electron-energy states in our full expression (21) for $\rho_1(E)$. Written in reduced units these are

$$\rho_1^{SC}(\nu)=\rho_1^{Kane}(\nu)=\frac{m^{*3/2}E_Q^{1/2}}{4\pi^2\hbar^3}(\xi')^{1/4}e^{-\nu^2/4\xi'}D_{-3/2}\left(\frac{\nu}{\sqrt{\xi'}}\right), \tag{35}$$

$$\rho^{free}(\nu)=\frac{m^{*3/2}E_Q^{1/2}}{\sqrt{2}\pi^2\hbar^3}\sqrt{|\nu|}\,H(-\nu), \tag{36}$$

where $H(\nu)$ is the Heaviside step function. The resulting densities of states $\rho_1(E)$ from (7), ρ_1^{Kane} and ρ^{free}, are plotted in Figs. 6–9 for values of $\xi'=50$, 5, 0.5, and 0.05.

We note first that the numerical values of $\rho_1(E)$ in Figs. 6–9 obtained here for case 3 by minimizing $B(E)$ agree with the numerical values calculated using the minimum counting method by Halperin and Lax who also minimized $B(E)$. This provides an excellent point of contact with previous values of $\rho_1(E)$. This case shows an unphysical turn downward in $\rho_1(E)$ as ν decreases to $\nu\sim 0$ to 5, depending upon the value of ξ'. Cases 1 and 2, on the other hand, yield a $\rho_1(E)$ that continues to rise as ν decreases and $\rho_1(E)$ eventually intersects the Kane semiclassical density of states. Strictly, only case 1 has a foundation in principle—the Lloyd-Best variational principle. However, since case 2, based on minimizing $\rho_1(E)$, agrees well with case 1 it can be taken, by virtue of this agreement, as an excellent approximation to the Lloyd-Best variational principle.

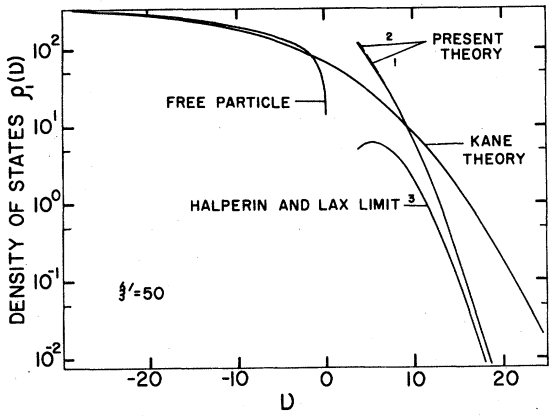

FIG. 6. Density of states

$$\rho_1(\nu,z)=\frac{Q^3}{E_Q\xi'^2}\,a(\nu,z)e^{-b(\nu,z)/2\xi'}$$

in units of $(Q^3/E_Q\xi'^2)$ for $\xi'=8\pi m^{*2}Z^2e^4\overline{N}/Q^5\hbar^4\epsilon_0^2=50$. The *present theory* is the band-tail value $\rho_1(E)$, Eq. (7), with the variational parameter z determined by (case 1) the Lloyd-Best variational principle, Eq. (11), and by (case 2) maximizing $\rho_1(E)$, Eq. (12). Case 1 and case 2 are indistinguishable at $\xi'=50$. The Halperin and Lax limit is $\rho_1(E)$ in Eq. (7) with z determined by minimizing the exponent in $\rho_1(E)$ (case 3). The Kane and free particle values are Kane's semiclassical result, (35) and (36), respectively.

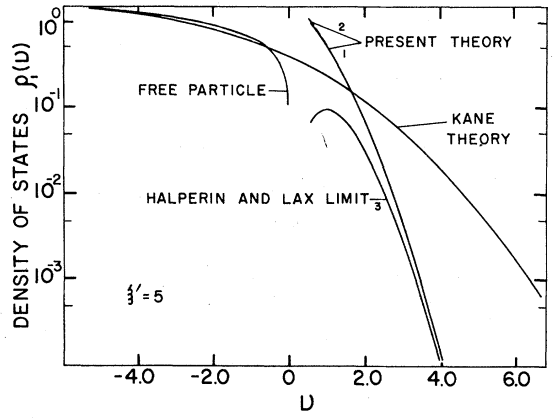

FIG. 7. As Fig. 6 for $\xi'=5$.

The results in Figs. 6–9 suggest an interpolation scheme for calculating the impurity-band density of states at all energies. In the band-tail region use $\rho_1(E)$ given by (7) with the variational parameter z determined from either of (11) or (12), since they give effectively the same final $\rho_1(E)$. This $\rho_1(E)$ should be used until it crosses the semiclassical Kane $\rho_1^{Kane}(E)$. Thereafter, for higher E use the $\rho_1^{Kane}(E)$. A similar matching of densities of states has been proposed by Thouless and Elzain.[28]

C. Corrections to $\rho_1(E)$

The band tail $\rho_1(E)$ in (7) was obtained from (21) in Sec. II and in I by retaining only the ground-state contributions to the density of states and by

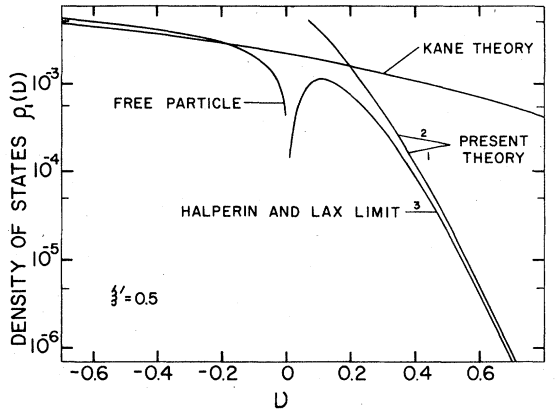

FIG. 8. As Fig. 6 for $\xi'=0.5$.

using the asymptotic expression of the parabolic cylinder function in (23). At high E some correction to $\rho_1(E)$ may be necessary. In the Appendix we estimate the leading correction to $\rho_1(E)$ from excited states. Including this leading correction and the leading correction in (23), we have

$$\rho_1^{\rm corr}(\nu)=\rho_1(\nu)\left(1-\frac{3}{16y^2}\right)\left\{1+\frac{4T}{(T+\nu)}\left(\frac{7T/3+\nu}{T+\nu}\right)^{5/2}y^2\exp\left[-y^2\frac{8}{9}\left(\frac{T}{T+\nu}\right)\left(\frac{5T+3\nu}{T+\nu}\right)\right]\right\}, \tag{37}$$

where $y^2=b(\nu,z)/2\xi'$. In (37) the correction $3/(16y^2)$ may be called the "deep-tail" correction since it is the correction to the asymptotic limit of the parabolic-cylinder function valid in the deep-tail region. The second correction in (37) involving T is the "excited-state" correction and $4T/3$ is, for example, the energy of the first excited state in units of E_Q. Clearly, for $\nu \gg T$, where y^2 is large, the corrections to $\rho_1(\nu)$ are negligible.

Halperin and Lax also evaluated a "deep-tail" correction. In their theory they retained only the leading term in a determinant in the deep-tail limit. By evaluating the whole determinant they obtained the "deep-tail" correction to be $3/2y^2$, a factor of 8 larger than ours. This difference of 8 probably enters from their approximate evaluation of the mean determinant appearing in their theory (see Sec. 7D, Ref. 2). They then set the limit of validity of $\rho_1(\nu)$ at $y^2 \geq 3$, at which point they obtained a deep-tail correction of $\frac{1}{2}$ or 50%. We believe the correction should be only $\frac{50}{8}=6.2\%$ at $y^2=3$. Halperin and Lax also estimated that the excited-state contributions would be small for $y^2 \geq 3$. Here we find that the excited-state contributions vanish for $\xi' \to 0$ where T becomes large (even at constant y^2), so a validity limit of a fixed value of y^2 may not be the most appropriate.

Since we wish to use $\rho_1(\nu)$ up to values of ν where it crosses the Kane-theory value, we evaluate the corrections to $\rho_1(\nu)$ in (37) at this energy. The value of ν at which the present theory $\rho_1(\nu)$ (cases 1 and 2) crosses $\rho^{\rm Kane}(\nu)$ depends upon ξ'. These ν values, obtained by equating $\rho_1(\nu)=\rho^{\rm Kane}(\nu)$, are shown in Fig. 10. For purposes of comparing with Halperin and Lax, the ratios $b(\nu,z)/2\xi'$ corresponding to these ν values are plotted in Fig. 11. This figure shows that the point at which $\rho_1(\nu)$ crosses $\rho^{\rm Kane}(\nu)$ is, interestingly enough, almost identical to the limit of validity $b(\nu,z)/2\xi' \approx 5$ for $\rho_1(\nu)$ selected by Halperin and Lax. Finally, in Fig. 12 the percentage correction to $\rho_1(E)$ at $\rho_1(\nu)=\rho^{\rm Kane}(\nu)$ is shown.

The leading correction to $\rho_1(E)$ due to excited states shown in Fig. 12 is positive and increases as ξ' increases. Physically, large ξ' corresponds to a broad impurity potential ($\xi' \propto Q^{-5}$). In this case the excited states will lie only slightly above the ground state and hence will be accessible and contribute to $\rho_1(E)$ at low E. At $\xi'=50$, the excited states still contribute less than 1% of $\rho_1(E)$.

The "deep-tail" correction $[-3/(16y^2)]$ in (37) from the leading term in (23) is negative and relatively independent of ξ'. This dominates the excited-state correction for all ξ' but does not exceed -5% of $\rho_1(E)$ at $\xi'=0.05$. If greater accuracy were required, the full parabolic-cylinder function as in (22) could be retained to calculate $\rho_1(E)$.

Hence we conclude that the deep tail $\rho_1(\nu)$ in (7) is correct to within 5% for ν values up to $\rho_1(\nu)=\rho^{\rm Kane}(\nu)$ for $0.05 \leq \xi' \leq 50$.

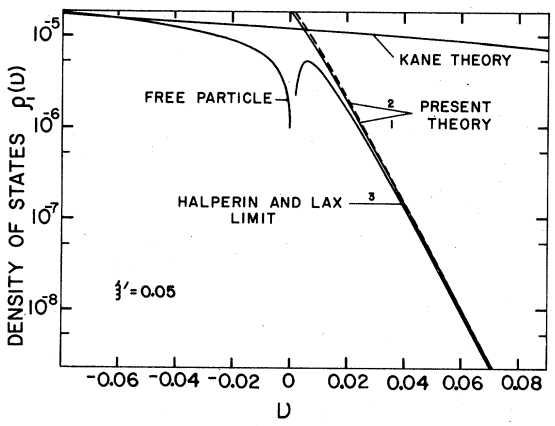

FIG. 9. As Fig. 6 for $\xi'=0.05$.

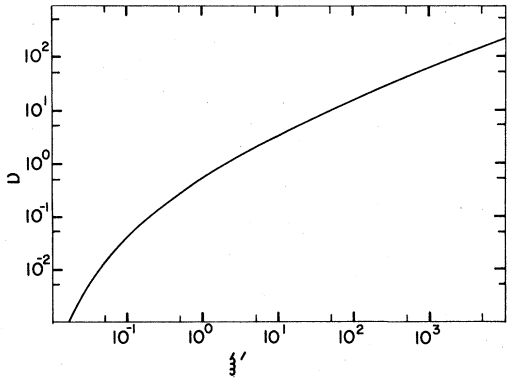

FIG. 10. Value of ν at which the *present theory* (case 1) $\rho_1(\nu)$ in (7) crosses the Kane semiclassical $\rho^{\rm Kane}(\nu)$ in (35), with z determined from (12).

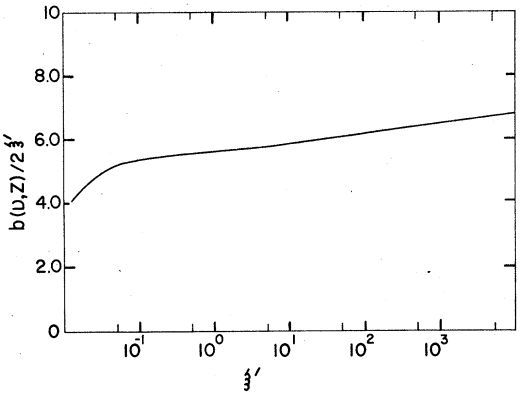

FIG. 11. Values of $b(\nu,z)/2\xi'$ at the point where $\rho_1(\nu) = \rho^{\text{Kane}}(\nu)$, with z determined from (12).

V. SUMMARY AND CONCLUSION

The central results of the present paper are shown in Figs. 6–9 as the *present theory* electron density of states in the impurity-band-tail region. This is obtained from Eq. (7) with the variational parameter z determined by solving (11) or (12). For small ξ' values the full Eq. (11), obtained from the Lloyd-Best variational principle, should be used to determine z.

The results in Figs. 6–9 suggest an interpolation scheme for calculating the impurity-band density of states in heavily doped semiconductors at all energies. In the band-tail region use the *present theory* $\rho_1(E)$ from the lowest energies up to the point at which it crosses the semiclassical Kane $\rho_1^{\text{Kane}}(E)$ given by (24) or (35). Thereafter, for higher E use the $\rho_1^{\text{Kane}}(E)$.

In future publications we plan to evaluate the full $\rho_1(E)$ given by (21) to check the proposed interpolation scheme and to apply the present results to calculation of band-tail parameters of heavily doped semiconductors. Also, in the limit of short-range potentials ($Q^{-1} \to 0$) the correlation function W in (4) and (5) reduces to a delta function (a white-noise potential). This limit has been studied extensively using the N-component Ginsburg-Landau model,[28-31] and explicit expressions for $\rho(E)$ in the band-tail region have now been obtained in three dimensions.[30,31] It would be interesting to explore in detail the relation between the present and the field-theoretic approaches.

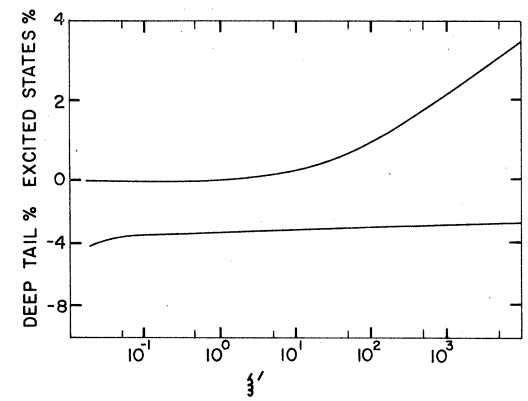

FIG. 12. Leading corrections to $\rho_1(\nu)$ due to the excited states and due to the "deep-tail" approximation [leading term in (23)] at $\rho_1(\nu) = \rho^{\text{Kane}}(\nu)$, with z determined from (12).

ACKNOWLEDGMENTS

It is a pleasure to acknowledge the invaluable contributions of the Canadian International Development Agency and of the Rachadapeseksompoch Research Fund toward this work.

APPENDIX

In Sec. II, the impurity-band-tail limit $\rho_1(E)$ in (7) was obtained from the full $\rho_1(E)$ in (21) by retaining only the ground-state contributions to $\rho_1(E)$ in (21). This was achieved by taking the $t \to \infty$ limit of the integrand in (21). Here we estimate the leading correction to (7) due to excited-state contributions.

In taking the $t \to \infty$ limit in (21) we use the following expansions:

$$\left(\frac{\omega t}{2\sin(\frac{1}{2}\omega t)}\right)^3 \simeq (i\omega t)^3 e^{-(3/2)i\omega t}(1+3e^{-i\omega t}), \tag{A1}$$

$$j(x,y)^{-3/2} \simeq \left(y+\frac{\hbar}{2m^*\omega}\right)^{-3/2} + \frac{3}{2}\left(\frac{\hbar}{2m^*\omega}\right)\left(y+\frac{\hbar}{2m^*\omega}\right)^{-5/2} \times (e^{-i\omega x}+e^{-i\omega(t-x)}-e^{-i\omega t}), \tag{A2}$$

$$\exp\{\tfrac{3}{2}[\omega t\cot(\tfrac{1}{2}\omega t)-1]\} \simeq e^{(3/4)i\omega t}(1+\tfrac{3}{2}i\omega t e^{-i\omega t}). \tag{A3}$$

These expansions hold for $t \to \infty$ provided t has a small negative imaginary part[19] ($t = t - i\epsilon$). The ground-state contribution to (21) is obtained by retaining only the first term in each of the expansions (A1), (A2), and (A3). At $t \to \infty$ the leading correction for the excited state comes from the second term in (A3) since it is proportional to t. [Strictly, the second term in (A2) is also proportional to t when substituted into (21) but it is also proportional to ξ', which is small in the deep-tail region.]

On substituting the first term of each of (A1), (A2), and (A3) in (20) we obtain

$$\rho_1(E)=\frac{1}{\pi\hbar}\,\mathrm{Re}\int_0^\infty dt\left(\frac{m^*}{2\pi i\hbar t}\right)^{3/2}(i\omega t)^3\exp\left[-\tfrac{3}{4}i\omega t-\frac{i}{\hbar}(E_0-E)t-\frac{\xi_Q Q t^2}{2\hbar^2\sqrt{\pi}}\int_0^\infty dy\, y e^{-Q^2 y}\left(y+\frac{\hbar}{2m^*\omega}\right)^{-3/2}\right]. \quad \text{(A4)}$$

The integration over y can be performed using the expression

$$\int_0^\infty dy\, y^{p-1}(y+\alpha)^{-p+1/2}e^{-\mu y} = 2^{p-1/2}\Gamma(p)\mu^{-1/2}e^{\alpha\mu/2}D_{1-2p}(\sqrt{2\alpha\mu}), \quad \text{(A5)}$$

where for the case above $p=2$, $\alpha=\hbar/2m^*\omega$, and $\mu=Q^2$. This gives

$$\rho_1(E)=\frac{1}{\pi\hbar}\,\mathrm{Re}\int_0^\infty dt\left(\frac{m^*}{2\pi i\hbar t}\right)^{3/2}(i\omega t)^3 e^{-\beta^2t^2-iqt}, \quad \text{(A6)}$$

where

$$\beta^2=\sqrt{2/\pi}\,\frac{\xi_Q}{\hbar^2}\,e^{z^2/4}D_{-3}(z) \quad \text{(A7)}$$

and

$$q=(\tfrac{3}{4}\hbar\omega+E_0-E)/\hbar. \quad \text{(A8)}$$

Finally, the integration over t can be done using

$$\int_{-\infty}^\infty dt(it)^{3/2}e^{-\beta^2t^2-iqt}=\frac{\sqrt{\pi}}{2^{3/4}}\,\beta^{-5/2}e^{-q^2/8\beta^2}D_{3/2}\left(\frac{q}{\sqrt{2}\beta}\right), \quad \text{(A9)}$$

which leads directly to (21) for the ground-state value of $\rho_1(E)$, where $b(\nu,z)/\xi'=\frac{1}{2}(q/\beta)^2$.

The first correction due to excited states is obtained by keeping the $\frac{3}{2}i\omega te^{-i\omega t}$ term in (A3) in place of the unit term. The $e^{-i\omega t}$ factor can be added to $\exp[-\frac{3}{4}i\omega t-(i/\hbar)(E_0-E)t]$ in (A4) and the y integration performed as before. In the t integration we now have

$$\int_0^\infty dt(it)^{5/2}e^{-\beta^2t^2-iq't}=\frac{\sqrt{\pi}}{2^{5/4}}\,\beta^{-7/2}e^{-q'^2/8\beta^2}D_{5/2}\left(\frac{q'}{\sqrt{2}\beta}\right)$$

in place of (A9). Hence the ratio of the leading excited-state to ground-state contribution to $\rho_1(E)$ is

$$R=\frac{3\omega}{2\sqrt{2}\beta}\,\frac{e^{-q'^2/8\beta^2}}{e^{-q^2/8\beta^2}}\,\frac{D_{5/2}(q'/\sqrt{2}\beta)}{D_{3/2}(q/\sqrt{2}\beta)} \quad \text{(A10)}$$

and

$$\rho_1^{\mathrm{Corr}}(E)=\rho_1(E)(1+R). \quad \text{(A11)}$$

Again using $b(\nu,z)/\xi'=\frac{1}{2}(q/\beta)^2$ and defining

$$b'(\nu,z)/\xi'\equiv\tfrac{1}{2}(q'/\beta)^2=\frac{b(\nu,z)}{\xi'}\,\frac{(T+4T/3+\nu)^2}{(T+\nu)^2} \quad \text{(A12)}$$

as well as going into the deep-tail limit, we have

$$R=\frac{3\omega b'(\nu,z)^{5/4}}{2\sqrt{2}\xi'\beta b(\nu,z)^{3/4}}\,e^{-(1/2\xi')[b'(\nu,z)-b(\nu,z)]}. \quad \text{(A13)}$$

Note here that in (A12), $4T/3=\hbar\omega/E_Q$ is the first-excited-state energy in reduced units. Expressed in terms of T and ν, we have

$$R=\frac{4T}{(T+\nu)}\left(\frac{7T/3+\nu}{T+\nu}\right)^{5/2}y^2 \times\exp\left[-y^2\frac{8}{9}\left(\frac{T}{T+\nu}\right)\left(\frac{5T+3\nu}{T+\nu}\right)\right], \quad \text{(A14)}$$

where $y=b(\nu,z)/2\xi'$.

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