Impurity-band density of states in heavily doped semiconductors: Numerical results

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The "band-tail" density of states $\rho(E)$ available to electrons in a field of randomly distributed, attractive impurities developed in previous work is extended to higher energy E. Numerical values of $\rho(E)$ are also presented (1) for comparison with $\rho(E)$ developed by other methods and (2) for calculation of optical and other properties of heavily doped semiconductors depending on $\rho(E)$.

I. INTRODUCTION

In earlier work[1] we obtained an expression for the density of states $\rho(E)$ available to electrons in a solid containing a high concentration of randomly distributed, attractive impurities. Of special interest is the value of $\rho(E)$ at low-energy E where $\rho(E)$ has an exponential tail extending deep into the gap between the conduction and valence band. To obtain an explicit, relatively simple expression for $\rho(E)$ valid at low E we made two approximations to the general expression. Firstly, only contributions to $\rho(E)$ from the electron ground states were retained. Secondly, the parabolic cylinder function $D_{3/2}$ was approximated by its large argument (deep-tail energy) limit. The $\rho(E)$ then reduced exactly to the form derived by Halperin and Lax.[2] The second approximation, which we call the "deep-tail" approximation, particularly limited the validity of $\rho(E)$ to the low-energy, deep-tail region of impurity-band energies.

Here we investigate to what extent these two approximations can be removed and how high an energy out of the band tail the $\rho(E)$ can be extended. We find that the "deep-tail" approximation can be quite easily removed. This allows us to improve the accuracy of and to extend $\rho(E)$ to somewhat higher energies. The contributions to $\rho(E)$ from excited states are, however, much more difficult to include and now set the limit of validity of $\rho(E)$. We also take this opportunity to present some numerical values for $\rho(E)$ which we hope will be useful in explicit calculations of properties of heavily doped semiconductors and in making comparisons

with $\rho(E)$ determined by other methods such as field-theoretic techniques.[3]

II. THE DENSITY OF STATES

A. The full ground-state density

In previous papers[1,4] the density of states for otherwise free electrons having effective mass m^* in a field of N random impurities (density $\bar{N}=N/\Omega$) with each impurity represented by a screened Coulomb potential

$$v(\vec{r}-\vec{R})=-\frac{Ze^2}{\epsilon_0|\vec{r}-\vec{R}|}e^{-Q|\vec{r}-\vec{R}|} \qquad (1)$$

was found to be

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

This result includes the ground states available to the electrons only; contributions to $\rho_1(v)$ from excited states have been ignored. In $\rho_1(v)$ all energies are expressed in units of $E_Q=\hbar^2Q^2/2m^*$, the energy associated with the screened impurity potential having screening length Q^{-1} in a medium having dielectric constant ϵ_0. The ξ' is the reduced-mean-square fluctuation of the random potential

$$\xi'=\xi_Q/E_Q^2=\frac{8\pi m^{*2}Z^2e^4\bar{N}}{\hbar^2\epsilon_0^2Q^5}, \qquad (3)$$

and $a(v,z)$ and $b(v,z)$ are functions

$$a(v,z)=(T+v)^{3/2}\bigg/\left[8\pi\sqrt{2}z^6\exp\left[\frac{z^2}{2}\right]D^2_{-3}(z)\right] ,$$

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

where $v=-(E-E_0)/E_Q$ is the electron energy E measured away from the mean of the random potential

$$E_0=\int d\vec{R}\,v(\vec{r}-\vec{R}) . \tag{5}$$

The $D_p(z)$ is the parabolic cylinder function and finally $z^{-2}=\frac{1}{2}\hbar\omega/E_Q$ is a free parameter setting the curvature ω of a model harmonic well which models the random potential. The optimum value of this parameter at each energy E may be determined from the variational principle derived by Lloyd and Best.[5] They showed that $\rho(v,z)$ should maximize the "pressure" function $P(v,z)$ given by

$$P(v,z)=E_Q^2\int_v^\infty dv'(v'-v)\rho(v,z) . \tag{6}$$

Maximizing $P(v,z)$ $[dP(v,z)/dz=0]$ leads to the equation for z,

$$\left[\frac{2}{z}-\frac{1}{4}\frac{D_{-4}(z)}{D_{-3}(z)}\right]\int_x^\infty dx'x'e^{-x'^2/4}D_{3/2}(x')$$

$$+\left[\frac{3}{4}\frac{D_{-4}(z)}{D_{-3}(z)}-\frac{2}{z}-\frac{z^{-3}}{T+v}\right]$$

$$\times\int_x^\infty dx'e^{-x'^2/4}D_{3/2}(x')=0 , \tag{7}$$

where

$$x=\left[\frac{b(v,z)}{\xi'}\right]^{1/2}$$

and $T=(\frac{3}{4})\hbar\omega/E_Q$ is the kinetic energy of electron localization.

B. The deep-tail approximation

In our previous determination,[1] referred to here as I, of $\rho_1(v,z)$, we approximated the parabolic cylinder function $D_{3/2}(x)$ in (2) by

$$D_{3/2}(x)=e^{-x^2/4}x^{3/2}\left[1-\frac{3}{8x^2}+\cdots\right] \tag{8}$$

and retained only the leading term. This is valid for large values of $x^2/2=b(v,z)/2\xi'$ which occur physically at large negative energies $E(v\gg1)$ deep in the band-tail energy region or at $\xi'\ll1$ and is denoted the "deep-tail" approximation. This led to the simpler equations in I for $\rho_1(v,z)$,

$$\rho_1(v,z)=\frac{Q^3}{E_Q\xi'^2}a(v,z)e^{-b(v,z)/2\xi'} \tag{9}$$

and the variational equation for z

$$\left[\frac{2}{z}-\frac{1}{4}\frac{D_{-4}(z)}{D_{-3}(z)}\right]\Gamma\left[\frac{7}{4},y\right]$$

$$+\left[\frac{3}{4}\frac{D_{-4}(z)}{D_{-3}(z)}-\frac{2}{z}-\frac{z^{-3}}{T+v}\right]y^{1/2}\Gamma\left[\frac{5}{2},y\right]=0 , \tag{10}$$

respectively. Here $\Gamma(\alpha,y)$ is the incomplete gamma function

$$\Gamma(\alpha,y)=\int_y^\infty dy'(y')^{\alpha-1}e^{-y'}$$

and

$$y=x^2/2=b(v,z)/2\xi' .$$

Equations (9) and (10) are identical to (7) and (11) in I. In I we found this approximation limited the energy range for $\rho_1(v,z)$ to low values of E. At values of E such that

$$x^2/2=b(v,z)/2\xi'\approx5$$

(a limit proposed by Halperin and Lax[2]) we found the leading correction $(3/8x^2)$ to $\rho_1(v,z)$ was approximately 4%, but we did not investigate higher terms or the effect of the approximation on the value of z determined from (10) rather than (7).

C. The Halperin and Lax limit

If we further take the limit $y\to\infty$ (valid at $\xi'\to0$) in $\Gamma(\alpha,y)$ and retain only the leading term in

$$\lim_{y\to\infty}\Gamma(\alpha,y)=y^{\alpha-1}e^{-y}\left[1+\frac{\alpha-1}{y}+\frac{(\alpha-1)(\alpha-2)}{y^2}+\cdots\right] ,$$

the Eq. (10) for z reduces to

$$\left[\frac{D_{-4}(z)}{D_{-3}(z)} - \frac{2z^{-3}}{(T+v)} \right] = 0 . \tag{11}$$

This is the limit considered by Halperin and Lax and obtained by them on the physical grounds of minimizing only the exponent $b(v,z)$ in (9).

III. NUMERICAL RESULTS

In Table I we present values of $\rho_1(v,z)$ and z in (1) the full ground-state case, (2) in the deep-tail approximation, and (3) in the Halperin and Lax limit. The Table shows firstly that the full ground-state density of states is smaller than the deep-tail approximation presented in I. The difference is displayed in Fig. 1 for $\xi' = 0.5$. The deep-tail approximation (8) is an expansion in $x^2/2 = b(v,z)/2\xi'$ valid at large $x^2/2$. At $b(v,z)/2\xi' \approx 5$ the deep-tail approximation lies $\sim 5\%$ above the full ground-state density. We take

this as the limit of validity of the deep-tail approximation. As noted in I, this is also the value of $b(v,z)/2\xi'$ at which $\rho_1(v,z)$ equals Kane's[6] classical density of states at each value of ξ'. The value of v and of $b(v,z)/2\xi'$ at which $\rho_1(v,z)$ crosses the Kane density of states as a function of ξ' is displayed in Figs. 2 and 3, respectively. In Fig. 3 we see the value of $b(v,z)/2\xi'$ at the crossing of $\rho^{Kane}(v)$ and $\rho_1(v,z)$ is smaller than the corresponding $b(v,z)/2\xi'$ in I. Since $\rho^{Kane}(v)$ is valid at high-energy E (small v) it was proposed to use $\rho_1(v,z)$ at low E (large v) and $\rho^{Kane}(v)$ at high E to obtain a density of states valid at all E. Over this range the deep-tail approximation to $\rho_1(v,z)$ presented in I will differ by less then 5% from the full ground-state $\rho_1(v,z)$.

Table I shows that the Halperin and Lax limit for $\rho_1(v,z)$ differs substantially from the full case at smaller values of v. If we again take a 5% difference as the validity domain, then the Halperin and Lax limit can be used for values of $b(v,z)/2\xi' \geq 10$.

The full case $\rho_1(v,z)$ itself neglects contributions

TABLE I. Numerical results for the density of states in units of $(Q^3/E_Q\xi'^2)$, at dimensionless energies v for the full ground-state case, the deep-tail approximation, and the Halperin and Lax limit.

ξ'	v	Halperin and Lax limit		Deep-tail approximation		Full ground-state case	
		z	$\rho(z)$	z	$\rho(z)$	z	$\rho(z)$
50	30	0.49225	6.8042×10^{-9}	0.43779	9.0368×10^{-9}	0.43778	8.9756×10^{-9}
	25	0.52264	4.7527×10^{-6}	0.45032	6.8394×10^{-6}	0.45030	6.7774×10^{-6}
	20	0.56237	1.1714×10^{-3}	0.46176	1.9166×10^{-3}	0.46171	1.8921×10^{-3}
	15	0.61805	9.2053×10^{-2}	0.46922	1.8939×10^{-1}	0.46907	1.8572×10^{-1}
	10	0.70592	1.9021×10^{0}	0.46684	6.3075×10^{0}	0.46640	6.1061×10^{0}
	5.0	0.88579	6.2013×10^{0}	0.44688	7.1360×10^{1}	0.44566	6.7319×10^{1}
	4.0	0.95289	5.5164×10^{0}	0.44047	1.0287×10^{2}	0.43902	9.6308×10^{1}
	3.0	1.0470	3.9975×10^{0}	0.43336	1.4309×10^{2}	0.43165	1.3282×10^{2}
5.0	3.0	1.0470	2.6584×10^{-3}	0.82777	4.3885×10^{-3}	0.82750	4.2948×10^{-3}
	2.5	1.1113	1.0116×10^{-2}	0.83797	1.8876×10^{-2}	0.83752	1.8380×10^{-2}
	2.0	1.1956	3.0087×10^{-2}	0.84480	6.7536×10^{-2}	0.84404	6.5301×10^{-2}
	1.5	1.3138	6.5938×10^{-2}	0.84634	1.9973×10^{-1}	0.84506	1.9125×10^{-1}
	1.0	1.5009	9.4700×10^{-2}	0.84051	4.8771×10^{-1}	0.83841	4.6079×10^{-1}
	0.5	1.8870	6.3651×10^{-2}	0.82594	9.9142×10^{-1}	0.82266	9.1990×10^{-1}
	0.4	2.0324	4.9007×10^{-2}	0.82197	1.1194×10^{0}	0.81841	1.0343×10^{0}
	0.3	2.2377	3.3381×10^{-2}	0.81767	1.2559×10^{0}	0.81383	1.1552×10^{0}
0.05	0.030	5.0609	4.5491×10^{-7}	3.8488	5.1982×10^{-7}	3.8472	5.0806×10^{-7}
	0.025	5.4296	8.4189×10^{-7}	3.9669	9.8535×10^{-7}	3.9647	9.6064×10^{-7}
	0.20	5.9270	1.5219×10^{-6}	4.0999	1.8483×10^{-6}	4.0968	1.7963×10^{-6}
	.015	6.6540	2.6450×10^{-6}	4.2507	3.4211×10^{-6}	4.2462	3.3111×10^{-6}
	.010	7.8747	4.2469×10^{-6}	4.4225	6.2191×10^{-6}	4.4156	5.9862×10^{-6}
	.005	10.655	5.4329×10^{-6}	4.6176	1.1018×10^{-5}	4.6066	1.0526×10^{-5}
	.004	11.786	5.2897×10^{-6}	4.6594	1.2302×10^{-5}	4.6887	1.0351×10^{-5}
	.003	13.454	4.8317×10^{-6}	4.7021	1.3714×10^{-5}	4.6887	1.3051×10^{-5}

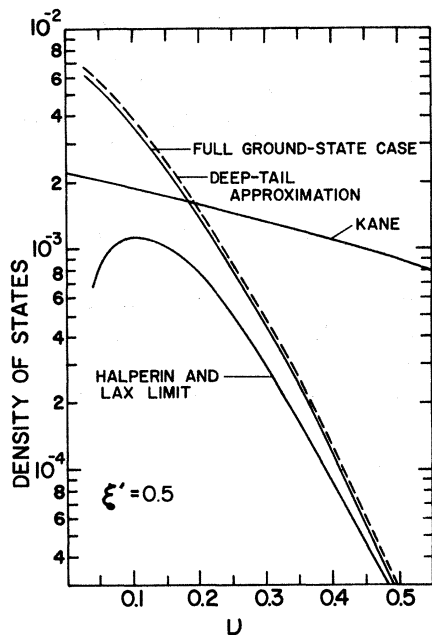FIG. 1. Density of states, in units of $(Q^3/E_Q\xi'^2)$, for the full ground-state case [Eq. (2)], for the deep-tail approximation [Eq. (9)], and for the Halperin and Lax limit [Eq. (9) with z determined by Eq. (11)]. Here ξ' in Eq. (3) is 0.5.

from excited states. We found these contributions much more difficult to evaluate or even approximate. The expression (2) for $\rho_1(v,z)$ is obtained by taking the infinite time limit in a long expression for $\rho_1(v,z)$ valid at all energies [Eq. (21) of I]. The infinite time limit means only ground states will be
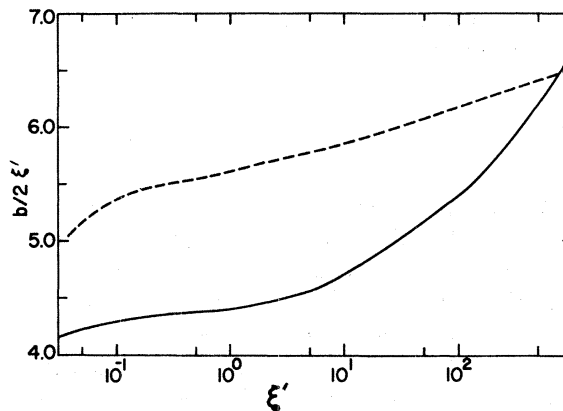

FIG. 3. As Fig. 2 for $b(v,z)/2\xi'$.

retained. Once this infinite time limit is not taken the expression for $\rho_1(v,z)$ is extremely difficult to evaluate and we have not been able to evaluate it at this time.

The leading corrections due to excited states can, however, be evaluated. Without making the deep-tail approximation there are two correction terms, given by (A2) and (A3) in I. The total correction depends strongly on ξ'. At $b(v,z)/2\xi'=4.3$, where $\rho_1(v,z)=\rho^{Kane}(v)$, the excited-state correction given by (A10) in I is less than 1% for $\xi'<5$. At $\xi'=500$ it is $\sim 3\%$. At large ξ' ($Q\rightarrow 0$) the potential (1) seen by the electrons becomes very broad and the excited states lie only slightly above the ground state. The dependence of the correction on ξ' at $b(v,z)/2\xi'$ for which $\rho_1(v,z)=\rho^{Kane}(v)$ is displayed in Fig. 4. Hence for $\xi'<50$ the excited-

FIG. 2. Value of v at which the full ground-state $\rho_1(v,z)$ [Eq. (2)] equals $\rho^{Kane}(v)$ (solid line) and the deep-tail approximation $\rho_1(v,z)$ [Eq. (9)] equals $\rho^{Kane}(v)$
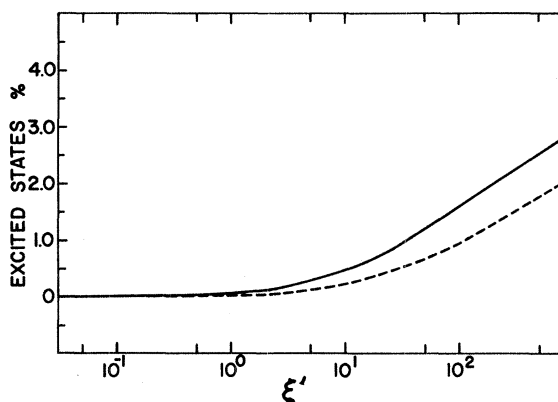

FIG. 4. Leading excited-state corrections to $\rho_1(v,z)$ evaluated at $\rho_1(v,z)=\rho^{Kane}(v)$; (1) full ground-state case

state correction is negligible for values of
$\rho_1(v,z) \leq \rho^{\text{Kane}}(v)$.

IV. CONCLUSION

We have presented numerical values of z and $\rho_1(v,z)$ for the full ground-state density of states, plus estimates of excited-state contributions. We hope these will be useful in calculations of optical and other properties of heavily doped semiconductors[7-10] and for explicit comparison with density-of-state expressions derived field theoretic and oth-

er techniques.[3] The field-theoretic studies usually consider δ-function potentials (1), which correspond approximately to $\xi' \to 0$. The density of states for a δ-function potential has also been evaluated using the present technique.[11]

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