Impurity-band tails based on semiempirical pseudopotentials in heavily doped semiconductors

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A new approximate method is presented for calculating the one-electron Green's function and the density of states for heavily doped semiconductors. The Green's function which was given by Bonch-Bruevich and by the present author under different approaches is used, but the true impurity potentials are replaced by semiempirical pseudopotentials giving an improved description of impurity-band tails. The theory is tested with the use of experimental data of the density of states in p-GaAs, showing considerable good agreement. In contrast, earlier theories turn out not to explain the experiments.

I. INTRODUCTION

Having useful expressions for a one-electron Green's function and impurity-band tails is of fundamental importance in analyzing various physical phenomena, e.g., tunneling, optical absorption, luminescence, conductivity, and Auger recombination, especially in heavily doped semiconductors. A number of calculations[1] based on perturbation and propagator techniques have led to tails that cut off sharply. It was shown[2] that perturbation methods are inadequate, especially in the tail. Kane[3] has calculated the density of states on the basis of the Thomas-Fermi approach for the potential-energy fluctuations, leading to Gaussian tail. This has been argued by Halperin and Lax[4] to be a disadvantage for the reason that simple exponential tails are often found. As the quantum counterpart of the semiclassical theory of Kane, Halperin, and Lax[4] have offered a minimum counting method, which is rigorous at sufficiently deep tail states. Sayakanit and Glyde[5] have improved the method with the aid of the variational principle. However, these two approaches are found to give poor descriptions of experimental data of tail states. On the other hand, Bonch-Bruevich[6] has discussed an approach based on the assumption that the potential varies slowly enough: Then the fluctuations in the energies of states mirror closely those in the potential energy. Instead of solving directly the differential equation, which was done by Bonch-Bruevich, the present author[7] has done the calculation using the diagram techniques, which are useful for the incorporation of other scattering effects such as phonon scattering effects. An approach of Bonch-Bruevich and the present author is frequently considered in this paper and is called the Bonch-Bruevich—Takeshima (BT) approach. In Ref. 7 the BT approach has been shown to explain well the experimental data of the conductivity in n-Ge but not that of the band-tail states of p-GaAs.

The assumption that effectively the potential varies slowly is useful in a heavy-doping range for states deep in the unperturbed band. For states around the band edge and in the band-gap region, however, the potential variation is no longer slow, even in an effective sense. As a result the fluctuations in the energies of states no longer mirror those in the potential energy. This paper shows that by using some appropriate potential, i.e., the pseudopotential, which is semiempirically determined, the BT approach is again useful. The pseudopotential is found analytically under two extreme conditions and by interpolation under intermediate conditions. On this basis the one-electron Green's function and the band-tail density of states are calculated for the band-gap region of practical interest as well as the region above the band edge.

II. MODEL AND BASIC FORMULATION

In this section we give the one-electron Green's function in a formal and complete form. First, we define our model by writing down the Hamiltonian as

$$H=\sum_{\vec{k}\sigma} E(\vec{k})a^{\dagger}_{\vec{k}\sigma}a_{\vec{k}\sigma}+\sum_{\vec{k}\vec{q}\sigma}\bar{\Gamma}(\vec{q})a^{\dagger}_{\vec{k}+\vec{q}\sigma}a_{\vec{k}\vec{\sigma}}, \tag{2.1}$$

where the first term and the second term are the Hamiltonians for the unperturbed band energy and the particle (electron or hole) impurity interaction, respectively. In the equation $a^{\dagger}_{\vec{k}\sigma}$, $a_{\vec{k}\sigma}$, and $E(\vec{k})$ are the creation operator, the annihilation operator, and the energy, respectively, for the particle with the wave vector $\vec{k}$ and the spin σ. The energy is mea-

sured from the relevant band edge so as to be positive and is given by

$$E(\vec{k})=\frac{\hbar^2}{2m^*}k^2 , \tag{2.2}$$

with m^* being the effective mass. $\bar{\Gamma}(\vec{q})$ is the Fourier component of $\Gamma(\vec{r})$, which is a sum of the screened impurity potentials $U(\vec{r}-\vec{R}_n)$ due to randomly distributed impurities located at $\vec{R}_n$, i.e.,

$$\Gamma(\vec{r})=\sum_{n=1}^{N_i} U(\vec{r}_n) , \tag{2.3}$$

where N_i is the total number of impurities and $\vec{r}_n=\vec{r}-\vec{R}_n$. Considering a single species of ionized impurities, we give

$$U(\vec{r}_n)=\frac{Ze^2}{\epsilon_0 r_n}\exp(-\lambda r_n) , \tag{2.4}$$

where Z is a positive or negative integer determined from both the sign of the particle charge and the valency of the impurity with respect to the host lattice, e the electronic charge, ϵ_0 the dielectric constant of the host lattice, and λ the Thomas-Fermi inverse screening length. For brevity we thus start only with the essential part of the Hamiltonian assuming the screening *a priori*. Discussions starting with the Hamiltonian including the unscreened electron-impurity, electron-phonon, and electron-electron interactions lead to the screened interactions, as has been given earlier.[7,8]

Now we consider the retarded Green's function,[9] which is derived from Eq. (2.1). In the presence of randomly distributed impurities the function is expressed in terms of two wave vectors $\vec{k}$ and $\vec{k}'$, one energy parameter ω, and the position vectors of randomly distributed impurities $\vec{R}_1, \vec{R}_2, \ldots, \vec{R}_{N_i}$ as $G^R(\vec{k},\vec{k}';\omega)$. Now we take an ensemble average[6,9,10] of $G^R(\vec{k},\vec{k}';\omega)$ over the impurity sites, which is defined as

$$\begin{aligned}\langle G^R(\vec{k},\vec{k}';\omega)\rangle &= \frac{1}{V^{N_i}}\int d\vec{R}_1 d\vec{R}_2 \ldots d\vec{R}_{N_i} G^R(\vec{k},\vec{k}';\omega) \\ &= G^R(\vec{k},\omega)\Delta(\vec{k}-\vec{k}') .\end{aligned} \tag{2.5}$$

Here $\Delta(x)$ is defined as $\Delta(x)=1$ if $x=0$ and $\Delta(x)=0$, otherwise with x as a scalar or a vector. The last step comes from the fact that the space uniformity, which is lost under random distribution of impurities giving $\vec{k}\neq\vec{k}'$, is restored under the average distribution giving momentum conservation $\vec{k}=\vec{k}'$. $G^R(\vec{k},\omega)$ is the retarded Green's function in the average impurity field, for which the rule of the diagram method is known. It was shown[11] that $G^R(\vec{k},\vec{k}';\omega)$ tends to $\langle G^R(\vec{k},\vec{k}';\omega)\rangle$ as $V\to\infty$.

In order to obtain the retarded Green's function $G^R(\vec{k},\vec{k}';\omega)$ we must solve the equation[9]

$$G^R(\vec{k},\vec{k}';\omega)=G_0^R(\vec{k},\omega)\times\left[\Delta(\vec{k}-\vec{k}')+\sum_{\vec{q}}\bar{\Gamma}(\vec{k}-\vec{q})G^R(\vec{q},\vec{k}';\omega)\right] . \tag{2.6}$$

Here $G_0^R(\vec{k},\omega)$ is the free-electron retarded Green's function

$$G_0^R(\vec{k},\omega)=\frac{1}{\omega+i\delta-E(\vec{k})} , \tag{2.7}$$

where $\delta\to 0^+$. Noting the relation

$$\Gamma(\vec{r})=\sum_{\vec{q}}\bar{\Gamma}(\vec{q})\exp(i\vec{q}\cdot\vec{r}) , \tag{2.8}$$

we obtain

$$\sum_{\vec{q}}\bar{\Gamma}(\vec{k}-\vec{q})G^R(\vec{q},\vec{k}';\omega) = \sum_{m=0}^{\infty}\frac{1}{m!}(i\nabla_k\cdot\nabla_r)^m\Gamma(\vec{r})G^R(\vec{k},\vec{k}';\omega)\,|_{\vec{r}=0} , \tag{2.9}$$

where $\nabla_k=\partial/\partial\vec{k}$ and $\nabla_r=\partial/\partial\vec{r}$. The symbolic solution to Eq. (2.6) reads

$$G^R(\vec{k},\vec{k}';\omega)=\frac{1}{\omega+i\delta-E(\vec{k})-\Gamma(i\nabla_k)}\times\Delta(\vec{k}-\vec{k}') . \tag{2.10}$$

The equation is rewritten as

$$G^R(\vec{k},\vec{k}';\omega) = \frac{1}{V}\int d\vec{r}\exp[i(\vec{k}-\vec{k}')\cdot\vec{r}]\times\frac{1}{\omega+i\delta-E(\vec{k}+i\nabla_r)-\Gamma(\vec{r})} . \tag{2.11}$$

This is the central equation from which the pseudopotential (ps) is found in the next section.

Let us assume that Eq. (2.11) can be rewritten as

$$G^R(\vec{k},\vec{k}';\omega) = \frac{1}{V}\int d\vec{r}\exp[i(\vec{k}-\vec{k}')\cdot\vec{r}]\times\frac{1}{\omega+i\delta-E(\vec{k})-\Gamma^{\rm ps}(\vec{r})} , \tag{2.12}$$

where $\Gamma^{ps}(\vec{r})$ is given by the pseudopotential $U^{ps}(\vec{r}_n)$ as

$$\Gamma^{ps}(\vec{r})=\sum_{n=1}^{N_i} U^{ps}(\vec{r}_n) . \tag{2.13}$$

According to the BT approach[7] where $\nabla_r=0$ is assumed in Eq. (2.11), $G^R(\vec{k},\omega)$ is directly found using Eqs. (2.12) and (2.13). It is to be noted that the analysis is useful under the condition that the imaginary part of the pseudopotential is zero or negative. The reason can be found from the derivation process in Ref. 7. Now we assume $U^{ps}(\vec{r})$ to be spherically symmetric. We must also consider the screened interaction between electrons at the positions $\vec{r}_1$ and $\vec{r}_2$,

$$U_e(\vec{r}_1-\vec{r}_2)=\frac{e^2}{\epsilon_0|\vec{r}_1-\vec{r}_2|}\times\exp(-\lambda|\vec{r}_1-\vec{r}_2|) . \tag{2.14}$$

It is convenient to define

$$h^{ps}(x)=\frac{\epsilon_0}{|Z|e^2\lambda}U^{ps}(\vec{r}) \tag{2.15}$$

and

$$h(x)=\frac{Z}{|Z|}\frac{\epsilon_0}{\epsilon^2\lambda}U_e(\vec{r}) , \tag{2.16}$$

where $x=\lambda r$. Then $G^R(\vec{k},\omega)$ is given as

$$G^R(k,\omega)=\frac{\epsilon_0}{|Z|e^2\lambda}\bar{G}^R(\Omega) , \tag{2.17}$$

$$\bar{G}^R(\Omega)=\frac{1}{i}\int_0^\infty d\xi\exp[i\xi\Omega+\gamma g(\xi)] , \tag{2.18}$$

$$g(\xi)=\int_0^\infty dx\, x^2\{\exp[-i\xi h^{ps}(x)]+i\xi h(x)-1\} , \tag{2.19}$$

$$\Omega=\frac{\epsilon_0}{|Z|e^2\lambda}[\omega-E(\vec{k})] , \tag{2.20}$$

$$h(x)=\frac{Z}{|Z|}\frac{1}{x}\exp(-x) , \tag{2.21}$$

$$\gamma=\frac{4\pi n_i}{\lambda^3} , \tag{2.22}$$

where $n_i=N_i/V$ is the impurity concentration. We will call the present analysis the pseudopotential (ps) approach hereafter. It is to be noted that the BT approach is the special case of the ps approach under $h^{ps}(x)=h(x)$. Assuming sufficiently large crystal volume, $G^R(\vec{k},\omega)$ is considered hereafter to offer the basis describing the physical phenomena in practical cases. If we want to incorporate some other scattering effects into the theory, we must only replace[7] $\omega-E(\vec{k})$ in Eq. (2.20) by $\omega-E(\vec{k})-\Sigma^R(\vec{k},\omega)$, where $\Sigma^R(\vec{k},\omega)$ is the self-energy arising from the scattering effects.

III. SEMIEMPIRICAL PSEUDOPOTENTIAL

In this section we find the pseudopotential starting with Eq. (2.11). Defining the operators

$$A=G_0^R(\vec{k},\omega)\Gamma(\vec{r}) , \tag{3.1}$$

$$B=G_0^R(\vec{k},\omega)O_p , \tag{3.2}$$

$$O_p=E(\vec{k}+i\nabla_r)-E(\vec{k}) , \tag{3.3}$$

$$T=\frac{1}{1-A-B} , \tag{3.4}$$

Eq. (2.11) is rewritten as

$$G^R(\vec{k},\vec{k}';\omega)=\frac{1}{V}G_0^R(\vec{k},\omega)\times\int d\vec{r}\exp[i(\vec{k}-\vec{k}')\cdot\vec{r}]T . \tag{3.5}$$

The special case of $B=0$ offers a basis for the BT approach, i.e.,

$$T=\frac{1}{1-A} . \tag{3.6}$$

Now we discuss the case of $B\neq 0$. Equation (3.4) is rewritten as

$$T=\frac{1}{1-A}\left[1+B\frac{1}{1-A}+B\frac{1}{1-A}B\frac{1}{1-A}+\cdots\right] . \tag{3.7}$$

We consider two extreme cases, $|A|\ll 1$ and $|A|\gg 1$. When $|A|\ll 1$, we obtain

$$T=1+A+BA+B^2A+\cdots=\frac{1}{1-\left[\frac{1}{1-B}A\right]} , \tag{3.8}$$

which is correct up to the first order in A for regions where $\Gamma(\vec{r})$ is continuous. In the equation, $[(1-B)^{-1}A]$ means that $(1-B)^{-1}$ operates on A only. Convergence of the series in the first step of Eq. (3.8), as well as the condition $|A|\ll 1$, is satisfied if $|\omega_k|$ is sufficiently large, where we define $\omega_k=\omega-E(\vec{k})$.

When $|A|\gg 1$, on the other hand, we must consider an additive restriction $|BA^{-1}|\ll 1$, noting that $(BA^{-1})^n$ $(n=1,2,\ldots)$ is independent of ω_k. Then we obtain

$$T=\frac{1}{1-A-A(BA^{-1})} , \tag{3.9}$$

which is correct up to the first order in both A^{-1} and BA^{-1}. In the equation, (BA^{-1}) means that B operates on A^{-1} only. Equations (3.8) and (3.9) show that the BT approach is useful if we replace A in Eq. (3.6) with $A^{\rm ps}$ given as follows:

$$A^{\rm ps}=\frac{1}{1-B}A \tag{3.10}$$

under $|A| \ll 1$ and

$$A^{\rm ps}=A+A(BA^{-1}) \tag{3.11}$$

under both $|A| \gg 1$ and $|BA^{-1}| \ll 1$. Evidently, $\Gamma^{\rm ps}(\vec{r})$ is obtained from

$$\Gamma^{\rm ps}(\vec{r})=[G_0^R(\vec{k},\omega)]^{-1}A^{\rm ps} .$$

First we consider the case $|A| \ll 1$. From Eqs. (2.13), (3.1), and (3.10) we obtain

$$U^{\rm ps}(\vec{r})=\frac{\omega_k}{\omega+i\delta-E(\vec{k}+i\nabla_r)}U(\vec{r}) . \tag{3.12}$$

Use of the Fourier expansion

$$U(\vec{r})=\frac{Ze^2}{2\pi^2\epsilon_0}\int d\vec{q}\,\frac{1}{q^2+\lambda^2}\exp(i\vec{q}\cdot\vec{r}) \tag{3.13}$$

gives

$$U^{\rm ps}(\vec{r})=\frac{Ze^2\omega_k}{2\pi^2\epsilon_0}\int d\vec{q}\,\frac{1}{q^2+\lambda^2}G_0^R(\vec{k}-\vec{q},\omega)\times\exp(i\vec{q}\cdot\vec{r}) . \tag{3.14}$$

For facility of later numerical analyses, we replace $E(\vec{k}-\vec{q})$ in $G_0^R(\vec{k}-\vec{q},\omega)$ by $E(\vec{k})+E(\vec{q})$, which offers a good approximation as far as k is sufficiently small. In practical calculations the range $|A| \ll 1$ is not important so that we may be satisfied with such crude evaluation. The integration of Eq. (3.14) can be easily performed. Using the definition (2.15) we obtain

$$h^{\rm ps}(x)=\frac{Z}{|Z|}\frac{\bar{\omega}_k}{\bar{\omega}_k+1}\frac{1}{x}\times[\exp(-x)-\exp(-q_0x)] \tag{3.15}$$

for $\omega_k<0$ and

$$h^{\rm ps}(x)=\frac{Z}{|Z|}\frac{\bar{\omega}_k}{\bar{\omega}_k+1}\frac{1}{x}\times[\exp(-x)-\exp(-iq_0x)] \tag{3.16}$$

for $\omega_k>0$, where $\bar{\omega}_k=\omega_k/(\hbar^2\lambda^2/2m^*)$ and $q_0=|\bar{\omega}_k|^{1/2}$. As stated in the preceding section, Eq. (3.16) is not appropriate for the pseudopotential since the imaginary part of $U^{\rm ps}(\vec{r})$ given from Eqs. (2.15) and (3.16) can be positive. Since the range $|A| \ll 1$ is not important in actual calculations of $\bar{G}^R(\Omega)$ and since Eq. (3.16) effectively agrees with Eq. (3.15) for $|\bar{\omega}_k| \gg 1$, we use Eq. (3.15) for $\omega_k>0$ as well as for $\omega_k<0$.

The condition $|A| \ll 1$ is expressed, by using Eq. (3.5) and the first step of Eq. (3.8), as

$$\left|\int d\vec{r}\exp[i(\vec{k}-\vec{k}')\cdot\vec{r}]\cdot\underline{1}\right| \gg \left|\int d\vec{r}\exp[i(\vec{k}-\vec{k}')\cdot\vec{r}]\cdot\underline{A}\right| .$$

Taking $\vec{k}=\vec{k}'$, we find that $|A| \ll 1$ corresponds to the condition

$$|\Omega| \gg \gamma . \tag{3.17}$$

Next we consider the case of $|A| \gg 1$ and $|BA^{-1}| \ll 1$. Let us write

$$A^{\rm ps}=G_0^R(\vec{k},\omega)[\Gamma(\vec{r})+\Gamma^r(\vec{r})] , \tag{3.18}$$

with

$$\Gamma^r(\vec{r})=\Gamma(\vec{r})O_p\frac{1}{\Gamma(\vec{r})} . \tag{3.19}$$

We obtain

$$\Gamma^r(\vec{r})=-\frac{\hbar^2}{2m^*}\left[2\left|\frac{\nabla_r\Gamma(\vec{r})}{\Gamma(\vec{r})}\right|^2-\lambda^2-i\frac{2\vec{k}\cdot\nabla_r\Gamma(\vec{r})}{\Gamma(\vec{r})}\right] . \tag{3.20}$$

Defining $\vec{x}_n=\lambda(\vec{r}-\vec{R}_n)$, we can write

$$|\nabla_r\Gamma(\vec{r})|^2=\left[\frac{Ze^2\lambda^2}{\epsilon_0}\right]^2\left[\sum_n\frac{1}{x_n^4}(1+x_n)^2\exp(-2x_n)+\sum_{n\neq n'}\frac{\vec{x}_n\cdot\vec{x}_{n'}}{x_n^3x_{n'}^3}(1+x_n)^2(1+x_{n'})^2\exp(-x_n-x_{n'})\right] . \tag{3.21}$$

Let x_l be the smallest of x_n's $(n=1,2,\ldots,N_i)$ and let r_0 be the radius of the average spherical volume per one impurity, i.e.,

$$\frac{4\pi}{3}r_0^3 n_i = 1 \ . \tag{3.22}$$

Then we may consider $x_l \lesssim x_0$ and $x_n \gtrsim x_0$ for $n \neq l$, where $x_0 = \lambda r_0$. Far outside the sphere of radius r_0, there may be a large number of x_n's with nearly equal magnitudes but various directions. These vectors $\vec{x}_n$ in a sum cancel out each other. As an approximation we assume that complete cancellation occurs for $\vec{x}_n$'s with $n \neq l$. Thus we neglect the second term in the second set of large parentheses in Eq. (3.21). The same consideration applies also to the last term in the large parentheses of Eq. (3.20). We obtain

$$\Gamma^r(\vec{r}) = -\frac{\hbar^2\lambda^2}{2m^*}\left[2\left|\frac{Ze^2\lambda}{\epsilon_0\Gamma(\vec{r})}\right|^2 \sum_n \frac{1}{x_n^4}(1+x_n)^2\exp(-2x_n) - 1 + \frac{i2Ze^2}{\epsilon_0\Gamma(\vec{r})}\frac{\vec{k}\cdot\vec{x}_l}{x_l^3}(1+x_l)\exp(-x_l)\right] . \tag{3.23}$$

From the equation we can find $U^{\rm ps}(\vec{r}_n)$ under the condition that $U^{\rm ps}(\vec{r}_n)$ should vanish in the limit of $r_n \to \infty$. However, this is only a formal result as far as $\Gamma(\vec{r})$ contained in the expression of $U^{\rm ps}(\vec{r})$ is not given. An approximate expression for $\Gamma(\vec{r})$ can be given under $x_0 \gtrsim 1$ or $x_0 \ll 1$. Under $x_0 \gtrsim 1$, $\Gamma(\vec{r})$ is nearly given by the impurity potential for $n = l$ only, while under $x_0 \ll 1$, $\Gamma(\vec{r})$ may be evaluated assuming uniform distribution of impurities. Here we consider the case of $x_0 > 1$ since this is found to be of practical interest. Then we can give

$$\Gamma(\vec{r}) = \frac{Ze^2\lambda}{\epsilon_0 x_l}\exp(-x_l) \ . \tag{3.24}$$

Writing $h^{\rm ps}(x_n)$ as

$$h^{\rm ps}(x_n) = h(x_n) + h^r(x_n) \ ,$$

where $h(x_n)$ given by Eq. (2.21) comes from $\Gamma(\vec{r})$ in Eq. (3.18), we obtain

$$h^r(x_l) = -\tfrac{1}{2}a_B\lambda\left[\frac{2}{x_l^2}(1+x_l)^2 - 1 - i\frac{2\vec{k}\cdot\vec{x}_l}{x_l^2}\right] \tag{3.25}$$

and

$$h^r(x_n) = -a_B\lambda\left[\frac{x_l}{x_n}\right]^2\frac{1}{x_n^2}(1+x_n)\exp(2x_l - 2x_n) \tag{3.26}$$

for $n \neq l$, where $a_B = \hbar^2\epsilon_0/(m^* e^2)$.

Equations (3.25) and (3.26) are understood to give $h^{\rm ps}(x)$ for $x \ll x_0$ and $x \gg x_0$, respectively. The last term in the large parentheses of Eq. (3.25) is neglected, noting that the case $x_l \simeq x_0$ is important: The term is small as far as x_0 is sufficiently large and/or k is sufficiently small. Equation (3.26) is evaluated using $x_l = x_0$. Giving $h^r(x)$, for the case intermediate between $x \ll x_0$ and $x \gg x_0$, by interpolation, we can construct the pseudopotential as

$$h^{\rm ps}(x) = h(x) + h^r(x) \ , \tag{3.27}$$

$$h^r(x) = -\frac{1}{2|Z|}\frac{a_B\lambda}{x^2[1+(x/x_0)]^2} \times \left[2(1+x)^2 - \exp\left[-\frac{x}{x_0}\right]\right] \times \exp\left[-\frac{2x^2}{x+x_0}\right] , \tag{3.28}$$

where $h(x)$ is defined by Eq. (2.21). In Eq. (3.27), $h(x)$ comes from $\Gamma(\vec{r})$ in Eq. (3.18), i.e., the true impurity potential. $h^r(x)$ is an additive term representing the situation in which the fluctuations in the energies of states do not mirror those in the potential energy. In fact, $h^r(x)$ vanishes in the limit of $a_B \to 0$ or $m^* \to \infty$, i.e., in the classical limit, under the condition that λ is a given constant. It is to be noted that $h^r(x)$ is always negative irrespective of the sign of Z, giving the attractive potential.

Now we discuss the conditions giving $|A| \gg 1$ and $|BA^{-1}| \ll 1$. Assuming uniform distribution of impurities for convenience, the condition for $|A| \gg 1$ leads to

$$|\omega_k| \ll |\Gamma(\vec{r})| = \left|n_i \int d\vec{R}\, U(\vec{r}-\vec{R})\right| , \tag{3.29}$$

giving

$$|\Omega| \ll \gamma \ . \tag{3.30}$$

The condition for $|BA^{-1}| \ll 1$ is rewritten as $|ABA^{-1}| \ll A$, i.e.,

$$|\Gamma(\vec{r})| \gg \left|\Gamma(\vec{r})O_p\frac{1}{\Gamma(\vec{r})}\right| .$$

With the use of the discussions similar to those for finding $h^{\rm ps}(x)$, the inequality is expressed as

$$\left|\int_0^\infty dx\, x^2 h(x)\right| \gg \left|\int_0^\infty dx\, x^2 h^r(x)\right| . \tag{3.31}$$

From this we obtain

$$1 \gg \frac{a_B\lambda}{|Z|}\phi(x_0) \ , \tag{3.32}$$

where

$$\phi(x_0)=\frac{1}{2}\int_0^\infty dx\frac{1}{(1+x/x_0)^2}\times\left[(1+x)^2-\exp\left[-\frac{x}{x_0}\right]\right]\times\exp\left[-\frac{2x^2}{x+x_0}\right]. \quad (3.33)$$

This function is shown in Fig. 1.

As a summary of this section the pseudopotential has been given by Eqs. (3.15) and (3.27) for $|\Omega|\gg\gamma$ and for $|\Omega|\ll\gamma$, respectively. In actual calculations we use Eqs. (3.15) and (3.27) for $|\Omega|>\Omega_c$ and for $|\Omega|<\Omega_c$, respectively, where Ω_c is determined empirically.

IV. NUMERICAL ANALYSES AND DISCUSSIONS

In this section discussions are given for states around the heavy-hole band of p-GaAs at 0 K as an example. The material parameters $\epsilon_0=12.79$ and $m^*/m_0=0.45$ are used, where m_0 is the electron mass in the free space. The attractive potential $Z=-1$ is considered. λ is calculated from $\lambda=[4k_F/(\pi a_M)]^{1/2}$, where k_F is the Fermi wave number given by $k_F=(3\pi^2 n_i)^{1/3}$ and a_M is the Bohr radius defined in terms of the effective mass of the band to which the majority carriers belong. Especially in the present case we have $a_M=a_B$.

First numerical calculations of $\mathrm{Im}\bar{G}^R(\Omega)$ are done for the case of $n_i=1.6\times10^{19}$ cm^{-3}. Figure 2 shows the result (—) obtained by taking $\Omega_c=5\gamma$ for the ps approach. For comparison the result (---) for the BT approach is shown. Both curves cut off sharply at $\Omega=\gamma$. This occurs as far as we have $h^{\mathrm{ps}}(x)<0$ for all the range of x, which is the present case. The reason is that $\mathrm{Im}\bar{G}^R(\Omega)$ is nonzero only in the range $\Omega<\gamma$, as has been discussed in Ref. 7. As a result $h^{\mathrm{ps}}(x)$ for $\Omega>\Omega_c$ is not necessary. At $\Omega=-\Omega_c$ ($\simeq-1.88$) the curve for the ps approach cuts off sharply, where $h^{\mathrm{ps}}(x)$ changes the expression from (3.27) to (3.15). It is to be noted that $h^{\mathrm{ps}}(x)$ for $\Omega<-\Omega_c$, i.e., Eq. (3.15), is much smaller in magnitude than the true impurity potential, i.e., $h(x)$, especially for small x. As a result $\mathrm{Im}\bar{G}^R(\Omega)$ becomes insignificant for $\Omega<-\Omega_c$. From the discussions above we see that a strict expression for $h^{\mathrm{ps}}(x)$ is not required in the range $|\Omega|>\Omega_c$.

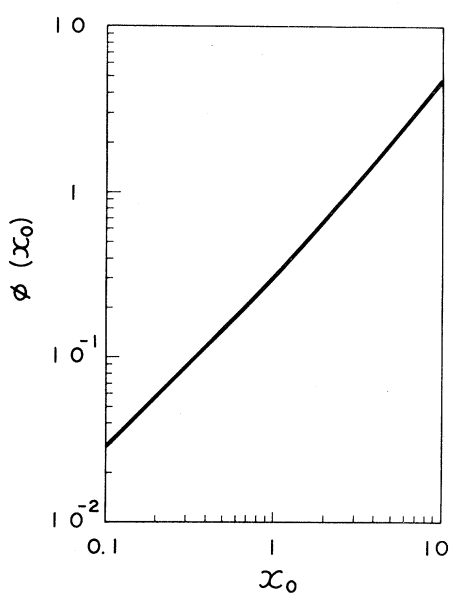

FIG. 1. $\phi(x_0)$ vs x_0 defined by Eq. (3.33).

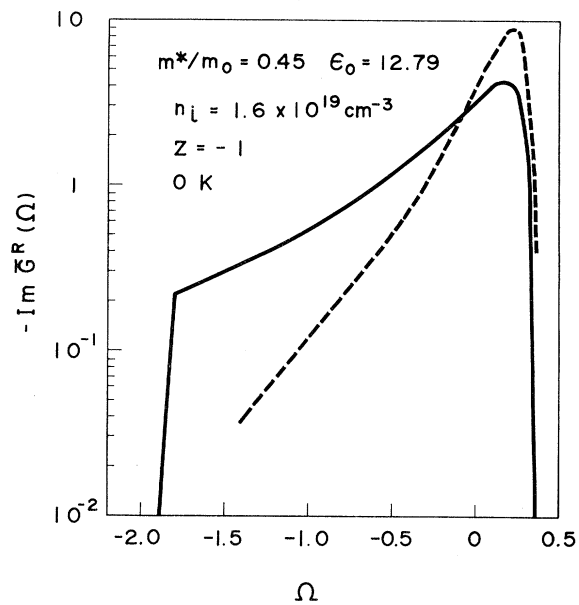

FIG. 2. $\mathrm{Im}\bar{G}^R(\Omega)$ calculated from the ps approach (—) and the BT approach (---).

Based on the results in Fig. 2, the density of states $\rho(\omega)$ is calculated from

$$\rho(\omega)=-\frac{2}{\pi}\int\frac{d\vec{k}}{(2\pi)^3}\mathrm{Im}G^R(\vec{k},\omega) \quad (4.1)$$

with the use of Eq. (2.17). Let $\rho^{\mathrm{ps}}(\omega)$ and $\rho^{\mathrm{ub}}(\omega)$ denote the densities of states obtained from the ps approach for the perturbed band and from the unperturbed parabolic band (ub) approach, respectively. For an energy state sufficiently deep in the unperturbed band the difference between $\rho^{\mathrm{ps}}(\omega)$ and $\rho^{\mathrm{ub}}(\omega)$ should be insignificant. Taking the requirement into account we have adopted $\Omega_c=5\gamma$, which gives a practically good agreement between $\rho^{\mathrm{ps}}(\omega)$

and $\rho^{ub}(\omega)$. Figure 3 shows the density of states (—) calculated with the use of the result of Fig. 2 for the ps approach. For comparison, results of the BT approach (—·—). Kane's approach[3] (----), and Halperin-Lax[4] and Sa-yakanit–Glyde[5] approaches (abbreviated as the HLSG approach) (—·) are also shown. It is to be noted that $n_i = 1.6\times10^{19}$ cm^{-3} gives $\xi' = 0.5$, where ξ' has been defined in the HLSG approach. In contrast with Kane's approach, which shows a Gaussian tail, the ps approach yields an exponential tail in the range where $\rho(\omega)$ is practically significant. Though the HLSG approach also gives an exponential tail, the tail cuts off much more rapidly for this approach than for the ps approach. It has been pointed out[4] that the HLSG approach is useful for the states which are too deep in the band-gap region and therefore too localized for adjacent wave functions to overlap. According to the criterion given in Ref. 4 the HLSG approach is useful in the range of $E \lesssim -0.02$ eV for the present case. However, from the discussion given in Ref. 4 we find that $E \ll -0.02$ eV may be a safe condition. This is the reason for the discrepancy between the HLSG approach and the ps approach.

Figures 4 and 5 show comparisons between the pseudopotential theory (—) and experiments[12] (○) on p-GaAs with $n_i = 5.4\times10^{18}$ cm^{-3} and 9.9×10^{18} cm^{-3}, respectively. The experimental plots of $\rho(\omega)$ around the heavy-hole band edge have been obtained from the tunneling experiments at 4.2 K. The calculations are done for 0 K. The screening parameter

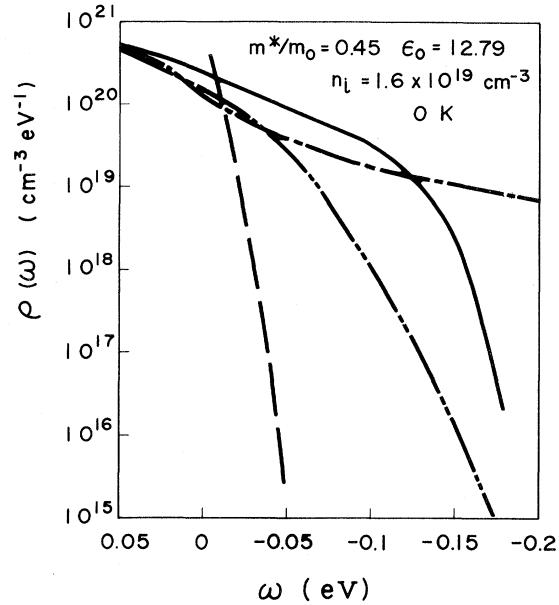

FIG. 3. Density of states $\rho(\omega)$ calculated from the ps approach (—), the BT approach (—·—), Kane's approach (----), and the HLSG approach (—·).

λ is calculated for simplicity assuming the unperturbed parabolic band. The experimental data are plotted in these figures so that an experimental value may fit the calculated value for the unperturbed band at a certain energy level lying deep in the band.

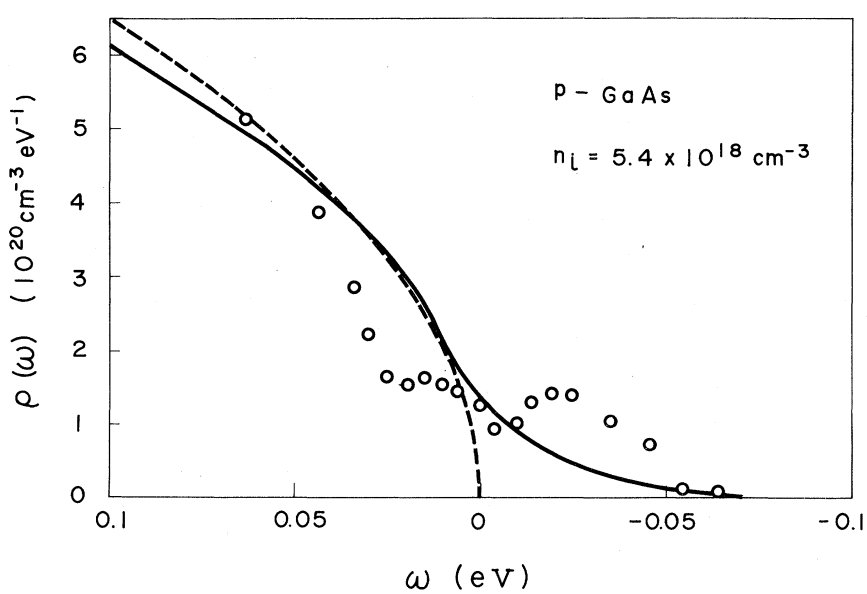

FIG. 4. Density of states $\rho(\omega)$ obtained from the ps approach (—), the unperturbed parabolic band approach (---), and the tunneling experiments at 4.2 K (○) (Ref. 12).

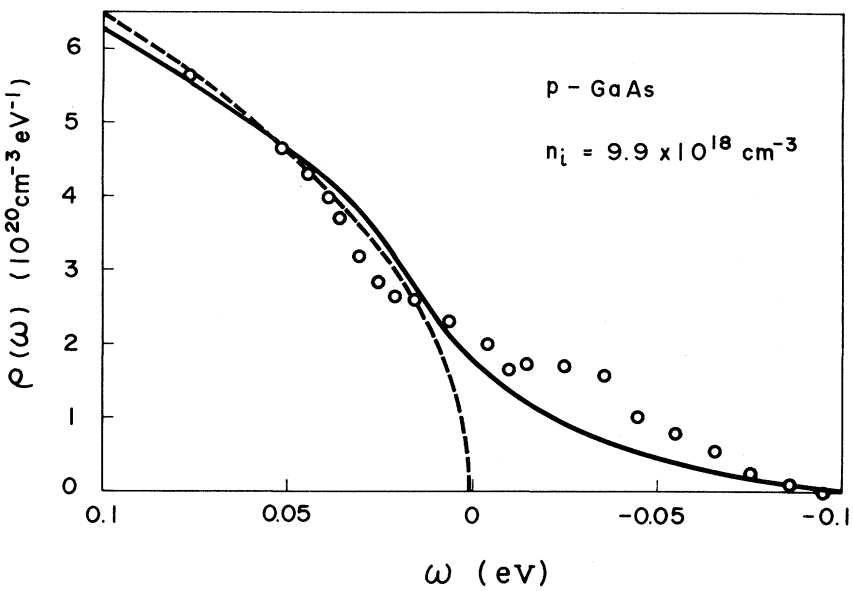

FIG. 5. Density of states $\rho(\omega)$ obtained from the ps approach (—), the unperturbed parabolic band approach (---), and the tunneling experiments at 4.2 K (○) (Ref. 12).

Considerably good agreements are found between the theory and the experiments. In contrast, the other approaches discussed in Fig. 3 cannot explain the experiments at all.

Let us consider the criterion (3.32), assuming degenerate statistics. We make use of an empirical relation $\phi(x_0)=0.3x_0^{1.2}$. From this we find that the criterion (3.32) is rewritten as $a_M n_i^{1/3} \gg 0.066 (a_B/a_M|Z|)^{10}$. Therefore, the ps approach is useful at heavy-doping levels. If we consider also the condition $x_0 \gtrsim 1$, the ps approach based on Eq. (3.28) is useful in the range

$$0.066\left[\frac{a_B}{a_M|Z|}\right]^{1/2} \ll a_M n_i^{1/3} \lesssim 1.5 . \tag{4.2}$$

Examination shows that this criterion is satisfied in the cases considered above. On the other hand, if states around the conduction-band edge in p-GaAs are considered, the ps approach cannot be used. In n-GaAs, states around the heavy-hole band edge can safely be analyzed by the present theory while those around the conduction-band edge should be analyzed under the condition $x_0 \lesssim 1$ as well as $x_0 \gtrsim 1$. Especially for $x_0 \ll 1$, $\Gamma(\vec{r})$ is given, in place of Eq. (3.24), by

$$\Gamma(\vec{r})=\frac{Ze^2\lambda}{\epsilon_0}\gamma , \tag{4.3}$$

assuming uniform distribution of impurities. As a result, Eqs. (3.28) and (3.33) should be replaced by

$$h^r(x)=-\frac{1}{2|Z|}\frac{a_B\lambda}{x^2(1+\gamma x)^2} \times[2(1+x)^2-\exp(-\gamma x)]\exp(-2x) \tag{4.4}$$

and

$$\phi(\gamma)=\tfrac{1}{2}\int_0^\infty dx\frac{1}{(1+\gamma x)^2} \times[2(1+x)^2-\exp(-\gamma x)]\exp(-2x) , \tag{4.5}$$

respectively. In conclusion, the pseudopotential analyses of the impurity-band tail states will offer a powerful tool for a comprehensive understanding of various physical phenomena in heavily doped semiconductors.

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