

Semiempirical pseudopotential approach to Green's-function formalism of electronic states in heavily doped semiconductors

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A semiempirical pseudopotential method is presented for calculating the electronic states in heavily doped semiconductors in terms of the one-electron Green's function. The present method is an improvement on the previously published one. The theory is tested using experimental data on *p*-type III-V compounds. It is shown that the impurity-band tails and the transport properties are well described by the present theory.

I. INTRODUCTION

Description of the electronic states in terms of the Green's function is a powerful tool for analyzing both optical and electrical properties of heavily doped semiconductors. The key factor affecting these properties is the impurity-band tail which appears as a result of the heavy doping. A number of earlier calculations¹ based on perturbation and propagator techniques have led to tails that are cut off sharply. Kane² has calculated the density of states with the use of the Thomas-Fermi approach for the potential fluctuation which has led to the Gaussian tail. A disadvantage of this method is that simple exponential tails are often observed experimentally.³ As the quantum counterpart of the semiclassical theory of Kane, Halperin and Lax³ have offered a minimum-counting method, which is rigorous for sufficiently deep states. Sa-yakanit and Glyde⁴ have improved the method with the aid of the variational principle. Let us hereafter call the approaches of Halperin-Lax and of Sa-yakanit-Glyde the HLSG approach. On the other hand, Bonch-Bruevich⁵ has discussed an approach based on the assumption that the potential varies slowly enough. Then the fluctuation in the energy of states mirrors closely that in the potential energy. Instead of solving directly the differential equation as was done by Bonch-Bruevich, this author did the calculation⁶ based on the diagram technique. The technique is useful for taking into account various effects such as the phonon scattering effect. Approaches by Bonch-Bruevich and this author are frequently considered in this paper and are called, hereafter, the Bonch-Bruevich-Takeshima (BT) approach. It has been pointed out⁷ that the HLSG approach and the BT approach offer the tail states that are cut off much more sharply than those which have been observed.

The assumption that the potential varies slowly enough is useful in a heavy-doping range for states deep in the unperturbed band. For states around the unperturbed 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 fluctuation in the energy of states no longer mirrors that in the potential energy. This is the weak point of the BT approach. A solution has been provided

by a pseudopotential approach which has been devised in a previous paper.⁷ In this approach the BT approach has been extended to include the effect of the rapidly varying potential with the use of an effective potential. This potential, named the pseudopotential, has been determined in a semiempirical manner and has been found to be useful for description of the band tails. However, a disadvantage of the above pseudopotential approach, called, hereafter, the previous ps approach, is that an unnatural cutoff must be provided for the Green's function in order to take into account the energy dependence of the pseudopotential. As a result we obtain the band tail that is cut off abruptly at a low energy. Another disadvantage is that the states around the unperturbed band edge cannot be described well. For instance, structures observed in the band tails, the conductivity data, and some of the Auger recombination data⁸ cannot be explained.

This paper presents an alternative semiempirical pseudopotential approach, called later the present ps approach, which extends the previous ps approach so as to include naturally the energy dependence of the pseudopotential. Unnatural cutoff of the band tail never appears and a wide range of the exponential tail is obtained. The observed structures of the band tails are reproduced quite well in the theory, especially at heavy-doping levels. The conductivity data for the doping range above the Mott transition are explained considerably well.

II. BASIC FORMULATION

In this section we describe briefly a formal but complete form of the one-particle Green's function for the states under the random distribution of impurities. A detailed discussion can be found in Ref. 7. In the presence of the randomly distributed impurities the retarded Green's function is given as a function of two wave vectors \vec{k} and \vec{k}' , one energy parameter ω , and the positions of the impurities $\vec{R}_1, \vec{R}_2, \dots, \vec{R}_{N_i}$; N_i is the number of the impurities in a crystal of volume V . We write the Green's function as $G^R(\vec{k}, \vec{k}'; \omega)$. Let $\Gamma(\vec{r})$ be a sum of the screened impurity potentials $U(\vec{r} - \vec{R}_n)$ due to the impurities located at \vec{R}_n , i.e.,

$$\Gamma(\vec{r}) = \sum_{n=1}^{N_i} U(\vec{r}_n), \quad (2.1)$$

where $\vec{r}_n = \vec{r} - \vec{R}_n$ and we consider a single species of the impurities. The unperturbed band energy at the wave vector \vec{k} is written as $E(\vec{k})$ and is measured from the band edge so as to be positive. Assuming the isotropic effective mass, we give $E(\vec{k}) = \hbar^2 k^2 / (2m^*)$. We obtain^{6,7}

$$G^R(\vec{k}, \vec{k}'; \omega) = \frac{1}{V} \int d\vec{r} \exp[i(\vec{k} - \vec{k}') \cdot \vec{r}] \times \frac{1}{\omega + i\delta - E(\vec{k} + i\vec{\nabla}_{\vec{r}}) - \Gamma(\vec{r})}, \quad (2.2)$$

where $\vec{\nabla}_{\vec{r}} = \partial/\partial\vec{r}$ and $\delta \rightarrow 0^+$.

Now we consider an ensemble average^{5,9,10} of $G^R(\vec{k}, \vec{k}'; \omega)$ over the impurity sites, which is defined as

$$\langle G^R(\vec{k}, \vec{k}'; \omega) \rangle = \frac{1}{V^{N_i}} \int d\vec{R}_1 d\vec{R}_2 \cdots d\vec{R}_{N_i} G^R(\vec{k}, \vec{k}'; \omega) = G^R(\vec{k}, \omega) \Delta(\vec{k} - \vec{k}'). \quad (2.3)$$

Here $\Delta(x)$ is defined as $\Delta(x) = 1$ if $x = 0$ and $\Delta(x) = 0$ otherwise, with x as a scalar or vector. The last step represents the fact that the space uniformity, which is lost under the random distribution of the impurities, is restored under the averaged 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.⁹ That $G^R(\vec{k}, \vec{k}'; \omega)$ tends to $\langle G^R(\vec{k}, \vec{k}'; \omega) \rangle$ as $V \rightarrow \infty$ has been shown in Ref. 11, where the impurity potentials screened in an exponential form have been assumed: The calculation is done hereafter for this case.

We assume that Eq. (2.2) can be rewritten as

$$G^R(\vec{k}, \vec{k}'; \omega) = \frac{1}{V} \int d\vec{r} \exp[i(\vec{k} - \vec{k}') \cdot \vec{r}] \frac{1}{\omega + i\delta - E(\vec{k}) - \Gamma^{\text{ps}}(\vec{r})}, \quad (2.4)$$

where $\Gamma^{\text{ps}}(\vec{r})$ is a sum of the pseudopotentials $U^{\text{ps}}(\vec{r}_n)$, i.e.,

$$\Gamma^{\text{ps}}(\vec{r}) = \sum_{n=1}^{N_i} U^{\text{ps}}(\vec{r}_n). \quad (2.5)$$

The BT approach starts with assuming $\vec{\nabla}_{\vec{r}} = \vec{0}$ in Eq. (2.2). Therefore Eq. (2.4) indicates that the result of the BT approach is directly useful by replacing $U(\vec{r})$ in the result with $U^{\text{ps}}(\vec{r})$. The analysis is useful under the condition that the imaginary part of the pseudopotential is zero or negative. The reason is found from the process of calculating $G^R(\vec{k}, \omega)$, given in Ref. 6.

Let us consider the ionized impurities of the valency Z

with respect to the host lattice. The many-body theoretical treatment of the electron-electron interaction leads⁶ to the screening of the Coulomb interactions between electrons and impurities as well as between electrons. We have

$$U(\vec{r}_n) = \frac{Ze^2}{\epsilon_0 r_n} \exp(-\lambda r_n), \quad (2.6)$$

where e is the electronic charge, ϵ_0 the static dielectric constant of the host lattice, and λ the inverse screening length. For λ we consider the Thomas-Fermi approach for simplicity. The interaction between electrons at \vec{r}_1 and \vec{r}_2 is given by

$$U_e(\vec{r}_1 - \vec{r}_2) = \frac{e^2}{\epsilon_0 |\vec{r}_1 - \vec{r}_2|} \exp(-\lambda |\vec{r}_1 - \vec{r}_2|). \quad (2.7)$$

It is convenient to define the dimensionless quantities

$$h^{\text{ps}}(x) = \frac{\epsilon_0}{|Z| e^2 \lambda} U^{\text{ps}}(\vec{r}) \quad (2.8)$$

and

$$h(x) = \frac{Z}{|Z|} \frac{\epsilon_0}{e^2 \lambda} U_e(\vec{r}) \quad (2.9)$$

with the use of $x = \lambda r$. Then $G^R(\vec{k}, \omega)$ in the pseudopotential approach is given as

$$G^R(\vec{k}, \omega) = \frac{\epsilon_0}{|Z| e^2 \lambda} \bar{G}^R(\Omega), \quad (2.10)$$

$$\bar{G}^R(\Omega) = \frac{1}{i} \int_0^\infty d\xi \exp[i\xi\Omega + \gamma g(\xi)], \quad (2.11)$$

$$g(\xi) = \int_0^\infty dx x^2 \{ \exp[-i\xi h^{\text{ps}}(x)] + i\xi h(x) - 1 \}, \quad (2.12)$$

$$\Omega = \frac{\epsilon_0}{|Z| e^2 \lambda} [\omega - E(\vec{k})], \quad (2.13)$$

$$h(x) = \frac{Z}{|Z|} \frac{1}{x} \exp(-x), \quad (2.14)$$

$$\gamma = \frac{4\pi n_i}{\lambda^3}, \quad (2.15)$$

where $n_i = N_i/V$ is the impurity concentration. In Sec. III we see that $h^{\text{ps}}(x)$ can be written in a form

$$h^{\text{ps}}(x) = h(x) + h^r(x). \quad (2.16)$$

Especially when we take $h^r(x) = 0$, we obtain the BT result. Our task in Sec. III is to find $h^r(x)$.

Equations (2.10)–(2.15) have been derived by considering the self-energy which includes all the terms of the electron-impurity interaction and the lowest-order Coulomb term of the electron-electron interaction with the free-particle Green's function being replaced by the perfect one. Let a sum of other self-energy terms be $\Sigma_{\text{res}}^R(\vec{k}, \omega)$. Then we should replace Ω in Eq. (2.11) by

$$\Omega - \frac{\epsilon_0}{e^2 \lambda} \Sigma_{\text{res}}^R(\vec{k}, \omega). \quad (2.17)$$

Although $G^R(\vec{k}, \omega)$ in Eqs. (2.10)–(2.15) is a function of Ω only, $G^R(\vec{k}, \omega)$ obtained under the replacement (2.17) is a function of \vec{k} and ω separately.

III. SEMIEMPIRICAL PSEUDOPOTENTIAL

In this section we seek out the pseudopotential starting with Eq. (2.2). Let us define the operators

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

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

$$O_p = E(\vec{k} + i\vec{\nabla}_{\vec{r}}) - E(\vec{k}), \quad (3.3)$$

$$T = \frac{1}{1 - A - B}, \quad (3.4)$$

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

$$G_0^R(\vec{k}, \omega) = \frac{1}{\omega + i\delta - E(\vec{k})}. \quad (3.5)$$

Equation (2.2) becomes

$$G^R(\vec{k}, \vec{k}'; \omega) = \frac{1}{V} G_0^R(\vec{k}, \omega) \int d\vec{r} \exp[i(\vec{k} - \vec{k}') \cdot \vec{r}] T. \quad (3.6)$$

It is convenient to rewrite Eq. (3.4) as

$$T = \frac{1}{1 - A} \left[1 + B \frac{1}{1 - A} + B \frac{1}{1 - A} B \frac{1}{1 - A} + \dots \right]. \quad (3.7)$$

The special case where the terms of the order higher than the zeroth in B are neglected, i.e.,

$$T = \frac{1}{1 - A}, \quad (3.8)$$

gives the BT approach. Therefore, we consider Eq. (3.7) as a series expansion of T with respect to the small perturbation $B(1 - A)^{-1}$. Especially up to the first order in $B(1 - A)^{-1}$ we obtain

$$\begin{aligned} T &= \frac{1}{1 - A} \left[1 + B \frac{1}{1 - A} \right] \\ &\approx \frac{1}{1 - A} \frac{1}{1 - B[1/(1 - A)]} \\ &\approx \frac{1}{1 - A - (1 - A)B[1/(1 - A)]}. \end{aligned} \quad (3.9)$$

Use of Eq. (3.9) in Eq. (3.6) and comparison of the obtained equation with Eq. (2.4) give

$$\Gamma^{\text{ps}} = \Gamma + (\omega_k - \Gamma) O_p \frac{1}{\omega_k - \Gamma + i\delta}, \quad (3.10)$$

where we define $\omega_k = \omega - E(\vec{k})$. We consider this equation as the basis of the pseudopotential approach. Since Eq. (3.10) is not useful at least for the case of $\omega_k - \Gamma = 0$,

we consider only the case of $\omega_k - \Gamma \neq 0$ and omit δ in the denominator. Let us define $\Omega_Z = (Z/|Z|)\Omega$, $x_n = \lambda |\vec{r} - \vec{R}_n|$, $\Gamma_x = \sum_{n=1}^{N_i} \exp(-x_n)/x_n$, and Γ_x' in terms of $\Gamma^{\text{ps}} = (e^2\lambda/\epsilon_0)(Z\Gamma_x + \Gamma_x')$. We obtain

$$\Gamma_x' = \frac{ia_B \vec{k} \cdot \vec{\nabla}_{\vec{x}} \Gamma_x}{\Omega_Z - \Gamma_x} - \frac{1}{2} a_B \lambda \left[\frac{\Gamma_x}{\Omega_Z - \Gamma_x} + 2 \frac{|\vec{\nabla}_{\vec{x}} \Gamma_x|^2}{(\Omega_Z - \Gamma_x)^2} \right], \quad (3.11)$$

where a_B is the Bohr radius defined by $a_B = \hbar^2 \epsilon_0 / (m^* e^2)$ and $\vec{\nabla}_{\vec{x}} \Gamma_x = \partial \Gamma_x / \partial \vec{x}$ with $\vec{x} = \lambda \vec{r}$. To neglect Ω_Z in the denominators offers the basis for the previous ps approach.⁶

We can write

$$\begin{aligned} |\vec{\nabla}_{\vec{x}} \Gamma_x|^2 &= \sum_{n=1}^{N_i} \frac{1}{x_n^4} (1 + x_n)^2 \exp(-2x_n) \\ &+ \sum_{n \neq n'} \frac{\vec{x}_n \cdot \vec{x}_{n'}}{x_n x_{n'}} (1 + x_n)^2 (1 + x_{n'})^2 \\ &\times \exp(-x_n - x_{n'}). \end{aligned} \quad (3.12)$$

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

$$\frac{4\pi}{3} r_0^3 n_i = 1. \quad (3.13)$$

Then we may have $x_l \leq x_0$ and $x_n \geq x_0$ 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. An approximation here is to assume that complete cancellation occurs on the second term of Eq. (3.12). The same consideration applies also to $\vec{k} \cdot \vec{\nabla}_{\vec{x}} \Gamma_x$ in Eq. (3.11) and we obtain $\vec{k} \cdot \vec{\nabla}_{\vec{x}} \Gamma_x = -\vec{k} \cdot \vec{x}_l \exp(-x_l)/x_l^3$. From Eqs. (2.5), (2.8), (2.16), (3.11), and the expression just above, we formally obtain

$$\begin{aligned} h^r(x_n) &= -\frac{a_B \lambda}{2|Z|} \left[\frac{1}{(\Omega_Z - \Gamma_x)^2} \frac{1}{x_n^4} (1 + x_n)^2 \exp(-2x_n) \right. \\ &\quad \left. + \frac{1}{\Omega_Z - \Gamma_x} \frac{1}{x_n} \exp(-x_n) \right] \\ &\quad - \frac{ia_B \vec{k} \cdot \vec{x}_l}{x_l^3} \exp(-x_l) \frac{1}{\Omega_Z - \Gamma_x} \delta_{nl}, \end{aligned} \quad (3.14)$$

where δ_{nl} is Kronecker's δ and Γ_x is given later as a function of x_n only. From Eq. (3.14) we should find $h^r(x)$. Unfortunately, however, we cannot do this on account of the Kronecker's δ on the last term. Moreover, this term can be positively imaginary so that the pseudopotential approach is not useful. For simplicity we omit that term noting that the term is not very important in the absolute magnitude.

Now we give Γ_x in the denominator of Eq. (3.14). Let us write

$$\begin{aligned}\Gamma_x &= \sum_{i=1}^{N_i} \frac{1}{x_i} \exp(-x_i) \\ &= \frac{1}{x_n} \exp(-x_n) + \Gamma'_{xn},\end{aligned}\quad (3.15)$$

where Γ'_{xn} is a sum of the potentials due to all the impurities except at \vec{R}_n , i.e.,

$$\Gamma'_{xn} = \sum_{i(\neq n)} \frac{1}{x_i} \exp(-x_i). \quad (3.16)$$

$$\begin{aligned}\Gamma_x &= \frac{1}{x_n} \exp(-x_n) + \gamma + \frac{\gamma}{2x_n} [(1-x_0) \exp(x_0-x_n) \theta(x_n-x_0) \\ &\quad + (1+x_0) \exp(x_n-x_0) \theta(x_0-x_n) - (1+x_0) \exp(-x_0-x_n)] \\ &\equiv u(x_n),\end{aligned}\quad (3.18)$$

where $\theta(x)=1$ for $x \geq 0$ and $\theta(x)=0$ otherwise.

As pointed out just below Eq. (3.10), Eq. (3.14) is not useful for $\Omega_Z - \Gamma_x = 0$. In order to suppress the divergence of $h'(x_n)$ we replace $\Omega_Z - \Gamma_x$ in Eq. (3.14) by $\Omega_Z - \Gamma_x + i\eta$ and take the real part of $h'(x_n)$ to be newly defined $h'(x_n)$. Here η is chosen to be a small positive quantity, which is determined empirically. We finally obtain

$$\begin{aligned}h'(x) &= -\frac{a_B \lambda}{2|Z|} \left[\frac{v(x)^2 - \eta^2}{[v(x)^2 - \eta^2]^2 + 4\eta^2 v(x)^2} \frac{(1+x)^2}{x^4} \right. \\ &\quad \times \exp(-2x) + \frac{v(x)}{v(x)^2 + \eta^2} \frac{1}{x} \\ &\quad \left. \times \exp(-x) \right],\end{aligned}\quad (3.19)$$

where

$$v(x) = \Omega_Z - \frac{1}{x} \exp(-x) - u(x). \quad (3.20)$$

It should be noted that $h'(x)$ diverges as x^{-2} for $x \rightarrow 0$ and vanishes as $\exp(-x)$ for $x \rightarrow \infty$. As a result the volume integral of $h'(x)$, i.e.,

$$\int d\vec{x} h'(x)$$

is finite. With the use of Eqs. (2.10)–(2.16) and the equations just above, the Green's function for the impurity scattering is obtained. Let us call this approach the present ps approach in contrast with the previous ps ap-

proach which has been referred to in Sec. I. A special case when we put $h'(x)=0$ is the BT approach.

$$\begin{aligned}\langle \Gamma'_{xn} \rangle &= \frac{1}{V^{N_i-1}} \\ &\times \int' d\vec{R}_1 d\vec{R}_2 \cdots d\vec{R}_{n-1} d\vec{R}_{n+1} \cdots d\vec{R}_{N_i} \Gamma'_{xn}.\end{aligned}\quad (3.17)$$

Here the prime on the integral symbol indicates that the integration over \vec{R}_i covers the range except the sphere of radius r_0 with center at \vec{R}_n : We have noted that $4\pi r_0^3/3$ is the average volume per one impurity. Thus Γ_x is divided into the potential due to the impurity at \vec{R}_n and the potentials due to the surrounding effective medium. For sufficiently large crystal volume V we obtain

proach which has been referred to in Sec. I. A special case when we put $h'(x)=0$ is the BT approach.

Now we consider the criteria under which the BT approach and the present ps approach are valid. The BT approach is the case in the classical limit: The potential change within one wavelength of a quantum particle should be sufficiently small, i.e., $2\pi\lambda/k \ll 1$ for a wave vector \vec{k} . From this condition it is clear that the BT approach is not useful for deep tail states where all \vec{k} states are important. Considering the special case where the important values of \vec{k} are around the Fermi wave vector for the unperturbed band, we replace k with k_F , where k_F is the magnitude of the Fermi wave vector. Actually, the requirement $2\pi\lambda/k_F \ll 1$ seems to be too strong and we may use $2\pi\lambda/(4k_F) \lesssim 1$ instead. On the other hand, the present ps approach is useful under the condition that the second term of Eq. (3.10) is a small correction. Thus from Eq. (2.16), the condition is expressed as $|h'(x)| \ll |h(x)|$ in an effective sense. Practically, this condition is rewritten as $a_B \lambda/2 \lesssim 1$, as is found from Eq. (3.19).

Let us restrict all the discussion hereafter to the case of 0 K for convenience. Considering in general multivalley semiconductors with valley number ν , we have $k_F = (3\pi^2 n_i / \nu)^{1/3}$ and $\lambda = [4\nu k_F / (\pi a_B)]^{1/2}$ on the unperturbed band model. Using these values we obtain the criteria

$$a_B n_i^{1/3} \gtrsim \nu^{4/3} \quad (3.21)$$

for the BT approach describing especially the states around the Fermi level and

$$a_B n_i^{1/3} \lesssim \nu^{-2/3} \quad (3.22)$$

for the present ps approach. It is seen that for $\nu=1$ all the range of n_i is covered by the BT approach and the present ps approach while for $\nu>1$ some range of n_i is covered by neither of these approaches.

In addition to the impurity scattering we consider the phonon scattering and the exchange energy. For the former we consider only the lowest-order diagram shown in Fig. 1. Taking into account the free carrier screening of the electron-phonon interaction, we obtain the self-energy Σ_{ep}^R at 0 K as¹²

$$\text{Re}\Sigma_{\text{ep}}^R(\vec{k}, \omega) = -\frac{2m^*}{\pi\hbar^2 k} \int_0^{q_B} dq q H_0(q) \ln \left| \frac{(k+q)^2 - q_0^2}{(k-q)^2 - q_0^2} \right|, \quad (3.23)$$

$$\text{Im}\Sigma_{\text{ep}}^R(\vec{k}, \omega) = -\frac{2m^*}{\hbar^2 k} [AH_1(k, q_0) + BH_2(k, q_0)],$$

which are useful for $\omega>0$. Here q_B is the Brillouin zone radius (assuming the spherical zone), $q_0 = (2m^*\omega/\hbar^2)^{1/2}$, $A = E_{\text{npo}}^2 \omega_{\text{op}} / (16\pi\bar{c})$, and $B = e^2 \omega_{\text{op}} / (4\epsilon^*)$,

$$H_0(q) = \frac{q^2}{(q^2 + \lambda^2)^2} (Aq^2 + B), \quad (3.24)$$

$$H_1(k, q_0) = 2kq_0 - \lambda^2 \left[\ln \left| \frac{(k+q_0)^2 + \lambda^2}{(k-q_0)^2 + \lambda^2} \right| - \frac{\lambda^2}{2} \left(\frac{1}{(k-q_0)^2 + \lambda^2} - \frac{1}{(k+q_0)^2 + \lambda^2} \right) \right], \quad (3.25)$$

$$H_2(k, q_0) = \frac{1}{2} \left[\ln \left| \frac{(k+q_0)^2 + \lambda^2}{(k-q_0)^2 + \lambda^2} \right| - \lambda^2 \left(\frac{1}{(k-q_0)^2 + \lambda^2} - \frac{1}{(k+q_0)^2 + \lambda^2} \right) \right]. \quad (3.26)$$

We have considered the nonpolar optical deformation potential scattering (the A terms) and the nonpolar optical



FIG. 1. Lowest-order diagram of the phonon scattering or of the exchange energy, where a dashed line represents the electron-phonon interaction or the electron-electron interaction, respectively; a full line represents the free-particle Green's function.

phonon scattering (the B terms); ω_{op} is the optical phonon energy, E_{npo} the optical deformation potential, \bar{c} the averaged elastic constant, and $(\epsilon^*)^{-1} = \epsilon_{\infty}^{-1} - \epsilon_0^{-1}$ with ϵ_{∞} as the high-frequency dielectric constant of the host lattice. For the exchange energy Σ_{ex}^R we consider only the term of the order lowest in the electron-electron interaction, as shown in Fig. 1 and replace the free-particle Green's function in the diagram by the perfect Green's function. We obtain

$$\Sigma_{\text{ex}}^R(\vec{k}, \omega) = \frac{e^2}{2\pi^2 \epsilon_0 k} \int_0^{\infty} dq q \ln \left| \frac{(k+q)^2 + \lambda^2}{(k-q)^2 + \lambda^2} \right| \times \int_{-\infty}^{\Omega_0} d\Omega \text{Im}\bar{G}^R(\Omega) \quad (3.27)$$

using the screened electron-electron interaction, where $\Omega_0 = [\omega_F - E(\vec{q})] \epsilon_0 / (e^2 \lambda)$ with ω_F as the Fermi level measured from the unperturbed band edge: Actually, we have used Eq. (2.10) as the perfect Green's function as an approximation.

As is seen from Eq. (2.11), $G^R(\vec{k}, \omega)$ is a function only of Ω in which \vec{k} and ω are included. This is an advantage from the viewpoint of the computation economy. However, the advantage is lost when we take into account $\Sigma_{\text{ep}}^R(\vec{k}, \omega)$ and $\Sigma_{\text{ex}}^R(\vec{k}, \omega)$. Actually, the effects of the phonon scattering and the exchange energy are not very important in the present paper. In view of this fact, we replace k in Eqs. (3.23)–(3.27) by k_F for simplicity and we have

$$\frac{\epsilon_0}{e^2 \lambda} E(\vec{k}) = \frac{3}{2} \gamma. \quad (3.28)$$

Writing

$$\omega = |Z| e^2 \lambda \Omega / \epsilon_0 + E(\vec{k}),$$

we also give

$$\omega = \frac{e^2 \lambda}{\epsilon_0} (|Z| \Omega + \frac{3}{2} \gamma). \quad (3.29)$$

Let us give the expression for the free carrier screening. As discussed in Ref. 6, the host-lattice plus free carrier screening constant $\epsilon(\vec{q})$ is given, neglecting the retardation effect, as

$$\epsilon(\vec{q}) = \epsilon_0 - \frac{4\pi e^2}{q^2} \chi(\vec{q}, 0), \quad (3.30)$$

where

$$\chi(\vec{q}, \omega) = -\frac{4}{\pi} \int \frac{d\vec{k}}{(2\pi)^3} [F(\vec{k}, \vec{q}; \omega) + F(\vec{k}, -\vec{q}; -\omega)] \quad (3.31)$$

with

$$F(\vec{k}, \vec{q}; \omega) = \int_{-\infty}^{\omega_F} d\omega' \text{Im}G^R(\vec{k}, \omega') \text{Re}G^R(\vec{k} + \vec{q}, \omega' + \omega). \quad (3.32)$$

Now we adopt the Thomas-Fermi approximation, i.e., take $\vec{q} \rightarrow 0$ in $\chi(\vec{q}, 0)$. We obtain

$$\begin{aligned} \lambda^2 &= -\frac{4\pi e^2}{\epsilon_0} \chi(0,0) \\ &= \frac{16\nu\sqrt{2\lambda'}}{\pi^2 a_B^{3/2}} \int_{-\infty}^{\Omega_F} d\Omega' \int_{-\infty}^{\Omega'} d\Omega (\Omega' - \Omega)^{1/2} \text{Im} G_{\lambda'}^R(\Omega) \\ &\quad \times \text{Re} G_{\lambda'}^R(\Omega), \end{aligned} \quad (3.33)$$

where $\Omega_F = \epsilon_0 \omega_F / (e^2 \lambda)$. Here the suffix λ' means that the relevant Green's function is obtained assuming a value λ' for the inverse screening length. Equation (3.33) provides iterative calculation: Using λ' a new value λ is obtained until sufficient convergence is attained.

The density of states $\rho(\omega)$ is obtained from

$$\rho(\omega) = -\frac{2}{\pi} \int \frac{d\vec{k}}{(2\pi)^3} \text{Im} G^R(\vec{k}, \omega), \quad (3.34)$$

which can be rewritten as

$$\begin{aligned} \rho(\omega) &= -\frac{\sqrt{2} m^* \nu}{\pi^3 \hbar^2} \left[\frac{|Z| \lambda}{a_B} \right]^{1/2} \\ &\quad \times \int_{-\infty}^{\Omega_\omega} d\Omega (\Omega_\omega - \Omega)^{1/2} \text{Im} \bar{G}^R(\Omega), \end{aligned} \quad (3.35)$$

where $\Omega_\omega = \epsilon_0 \omega / (e^2 \lambda)$. It is considered that $\rho(\omega)$ at $\omega \rightarrow \infty$ is just the value for the unperturbed band, i.e., $(2m^*/\hbar^2)^{3/2} \sqrt{\omega} / (2\pi^2)$. From this we obtain the relation

$$\int_{-\infty}^{\infty} d\Omega \text{Im} \bar{G}^R(\Omega) = -\pi \quad (3.36)$$

as the necessary condition a given approach should satisfy. In fact it is easy to show that the condition is satisfied for the BT approach. However, this cannot be shown analytically for the present ps approach. The numerical calculation shows that Eq. (3.36) holds approximately. The deviation of the calculated value of the left-hand side of Eq. (3.36) from the right-hand side value is small, i.e., within 10%. A correction is made by multiplying the obtained Green's function with a constant value so that the new Green's function may satisfy the condition (3.36).

The Fermi level ω_F is determined from the relation

$$n_i = \int_{-\infty}^{\omega_F} d\omega \rho(\omega). \quad (3.37)$$

The conductivity σ is given from Ref. 6 as

$$\sigma = \frac{\nu e^2 \hbar^3}{3\pi^3 (m^*)^2} \int_0^\infty dk k^4 [\text{Im} G^R(\vec{k}, \omega_F)]^2, \quad (3.38)$$

which is rewritten as

$$\begin{aligned} \sigma &= \frac{2\sqrt{2}\nu e^2}{3\pi^3 \hbar} \left[\frac{|Z| \lambda}{a_B} \right]^{1/2} \\ &\quad \times \int_{-\infty}^{\Omega_F} d\Omega (\Omega_F - \Omega)^{3/2} [\text{Im} \bar{G}^R(\Omega)]^2. \end{aligned} \quad (3.39)$$

IV. NUMERICAL ANALYSIS AND DISCUSSION

In this section the Green's function obtained in the preceding sections is tested. The discussion is restricted

hereafter to the case of 0 K and $Z = -1$; we assume one species of impurities and consider ionized donors and acceptors for the conduction band and for the valence band, respectively. The effects of the phonon scattering and the exchange energy are taken into account unless stated otherwise.

The value of η in Eq. (3.19) little affects calculated results if η is small, i.e., below unity. This is natural since the exponential term in Eq. (2.12) oscillates rapidly with x around the value giving $v(x) = 0$ and little contributes to the integration in this range of x . From this fact we can rather arbitrarily choose the value of η . In practice we use $\eta = 0.01$.

First we consider *p*-type GaAs, for which we use the heavy hole mass m_H as $m_H/m_0 = 0.48^{13}$ (m_0 is the electron mass in the free space), $\epsilon_0 = 12.79$,¹⁴ the phonon parameters given in Refs. 14 and 15, and $\nu = 1$. Figures 2 and 3 show the theoretical results and the experimental data on the density of states around the valence band on *p*-type GaAs with $n_i = 5.4 \times 10^{18} \text{ cm}^{-3}$ and $n_i = 9.9 \times 10^{18} \text{ cm}^{-3}$, respectively. These values of n_i satisfy the criterion (3.22) for the present ps approach: The criterion (3.22) is rewritten as $n_i \leq 3.6 \times 10^{20} \text{ cm}^{-3}$. The full lines and the dashed lines show the present ps results and the BT results, respectively. The open circles show the experimental plots,¹⁶ which have been obtained from the tunneling experiments at 4.2 K. The data are plotted so that an experimental point at an energy level lying deep in the band may fit the value calculated for the unperturbed band. The present ps approach well explains the experimental band tails in remarkable contrast with the BT approach. However, for the present ps approach the structures in the band tails are not so evident as the observed

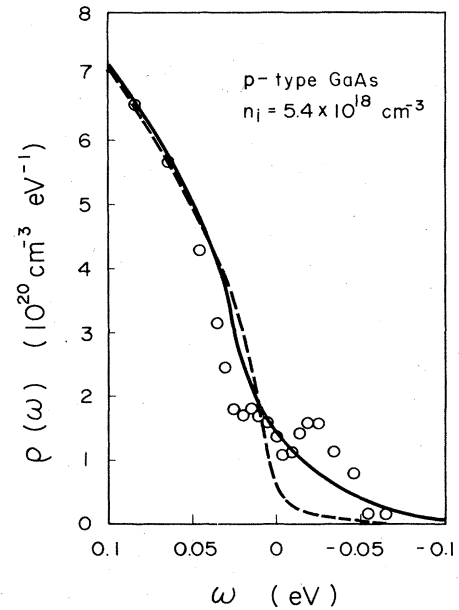


FIG. 2. Density of states around the valence band on *p*-type GaAs with $n_i = 5.4 \times 10^{18} \text{ cm}^{-3}$, where a full line, a dashed line, and open circles show the results of the present ps approach, the BT approach, and the experiments at 4.2 K, respectively.

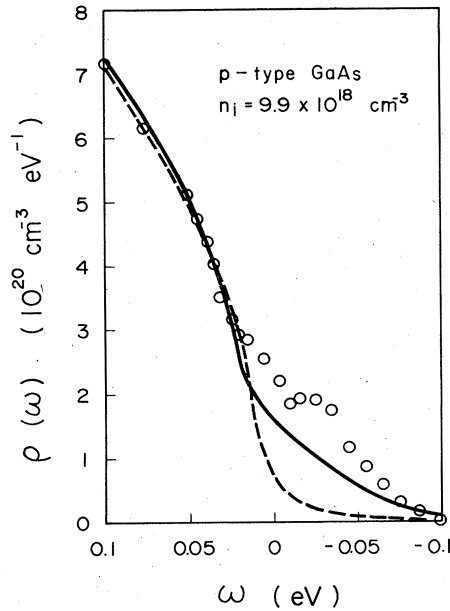


FIG. 3. Density of states around the valence band on *p*-type GaAs with $n_i = 9.9 \times 10^{18} \text{ cm}^{-3}$, where a full line, a dashed line, and open circles show the results of the present ps approach, the BT approach, and the experiments at 4.2 K, respectively.

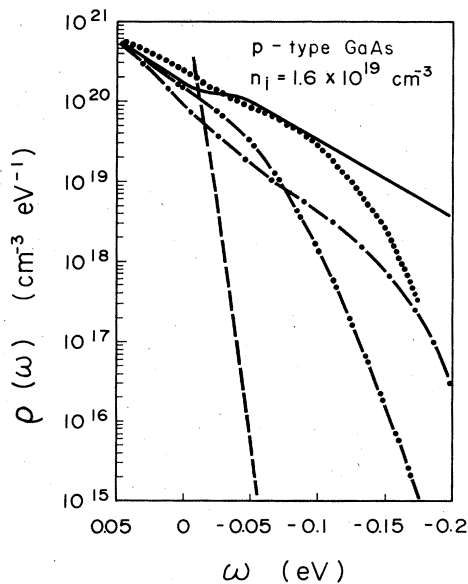


FIG. 4. Density of states around the valence band on *p*-type GaAs with $n_i = 1.6 \times 10^{19} \text{ cm}^{-3}$, which is calculated from the present ps approach (a full line), the previous ps approach (a dotted line), the BT approach (a dashed-dotted line), the Kane's approach (a dashed-double-dotted line), and the HLSG approach (a dashed line).

one in the impurity concentration range under consideration. The main cause for the discrepancy may be the ensemble average over the impurity sites which is taken over the Green's function. For the calculation of the full lines the effects of the phonon scattering and the exchange energy have been considered. The effects have been found to be negligible on the band tails, although the effects are not negligible on the conductivity ($\sim 10\%$).

Let us compare the present ps approach with various other approaches on *p*-type GaAs with $n_i = 1.6 \times 10^{19} \text{ cm}^{-3}$, which satisfies the criterion (3.22). Especially in this case use has been made of the inverse screening length for the unperturbed band and iteration has not been done although by the iteration λ is reduced by about 20%. Figure 4 shows the density of states calculated from the present ps approach (a full line), the previous ps approach⁷ (a dotted line), the BT approach (a dashed-dotted line), the Kane's approach (a dashed-double-dotted line), and the HLSG approach (a dashed line). The HLSG line is found from Ref. 4, giving the calculated result for $\xi' = 0.5$, the value of which corresponds to $n_i = 1.6 \times 10^{19} \text{ cm}^{-3}$. All the previous approaches except the previous ps approach give much smaller values of $\rho(\omega)$ in the band-gap region than does the present ps approach. That the present ps approach shows a structure a little below the unperturbed band edge agrees with the experimental facts (see Figs. 1 and 2) and is in contrast with the previous ps approach which gives a monotonous change of $\rho(\omega)$.

Figure 5 shows $\text{Im}\bar{G}^R(\Omega)$'s, which are calculated from the present ps approach (a full line), the previous ps approach (a dashed-dotted line), and the BT approach (a dashed line) on *p*-type GaAs with $n_i = 1.6 \times 10^{19} \text{ cm}^{-3}$. The effects of the phonon scattering and the exchange energy have not been considered. It is seen that the present ps approach gives a peak of $-\text{Im}\bar{G}^R(\Omega)$ for $\Omega \leq 0$ in contrast with both the previous ps approach and the BT approach. Considering that the existence of the peak is a

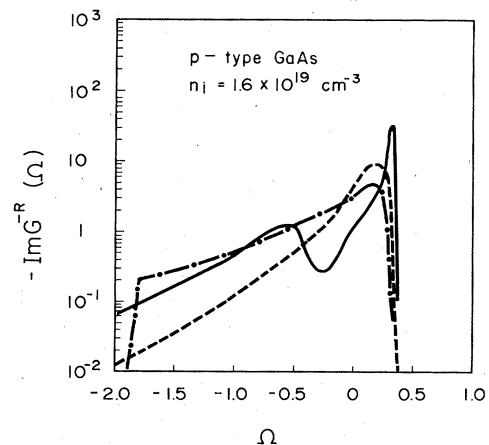


FIG. 5. $\text{Im}\bar{G}^R(\Omega)$ calculated from the present ps approach (a full line), the previous ps approach (a dashed-dotted line), and the BT approach (a dashed line).

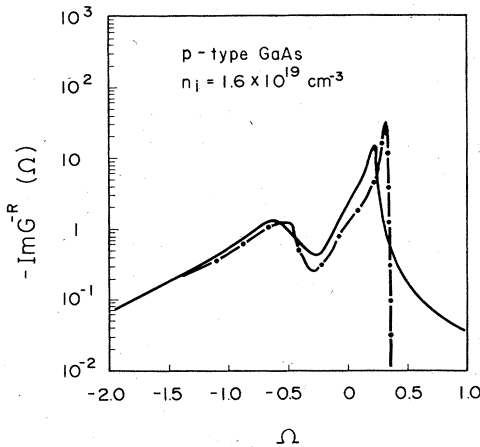


FIG. 6. $\text{Im}\bar{G}^R(\Omega)$ calculated from the present ps approach taking into account (a full line) and neglecting (a dashed-dotted line) the effects of the phonon scattering and the exchange energy.

prerequisite to giving the structure of $\rho(\omega)$, the present ps approach is more rigorous than the other two approaches. In the previous ps approach the cutoff of $\text{Im}\bar{G}^R(\Omega)$ is provided at $\Omega = -5\gamma$ so that the condition (3.36) may be satisfied. In contrast, this artificial cutoff is not necessary in the present ps approach.

Figure 6 shows $\text{Im}\bar{G}^R(\Omega)$ for the present ps approach, where the effects of the phonon scattering and the exchange energy are considered for the full line and not considered for the dashed-dotted line. The effects are seen to be unimportant at low values of Ω so that the band tails are little influenced by the effects. The effects are important especially around $\Omega = \gamma$. It is a purely analytical result⁶ that in the BT approach $\text{Im}\bar{G}^R(\Omega)$ is zero in the range $\Omega > \gamma$ unless the phonon scattering effect as well as the exchange energy effect is considered. Empirically, this is the case for the previous ps approach and for the present ps approach. The role of the exchange energy is to cause the energy shift toward the lower-energy region.

Let us consider the drift mobility μ of carriers, which is given from Eq. (3.39) as $\mu = \sigma / (n_i e)$. Figure 7 shows the theoretical results and the experimental data of μ on *p*-type GaP. The full line and the dashed line show the results of the present ps approach and the BT approach, respectively, which are obtained using $m_H/m_0 = 0.54$,¹³ $\epsilon_0 = 10.75$,¹⁴ and $\nu = 1$. The dashed-dotted line and the open circle show the experimental results at low temperatures (~ 4 K). The criterion (3.22) corresponds to $n_i \lesssim 1.0 \times 10^{21} \text{ cm}^{-3}$ so that the present ps approach is useful in the range of n_i where the experimental data are available. In fact, the value of μ shown by the open circle is explained by the present ps approach. The experiments

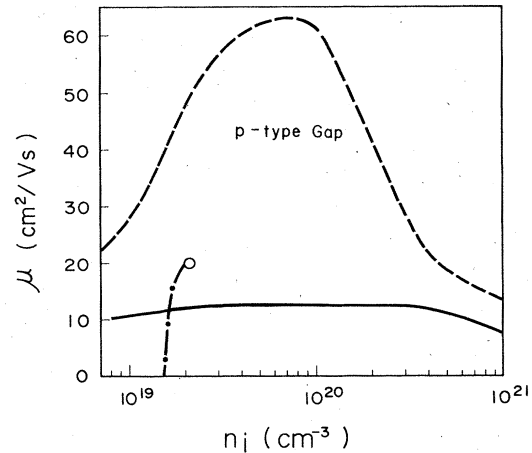


FIG. 7. Mobility μ vs n_i in *p*-type GaP, which is obtained from the present ps approach (a full line), the BT approach (a dashed line), and the experiments (an open circle and a dashed-dotted line).

show that the mobility change with n_i around 10^{19} cm^{-3} is very rapid. This suggests that the Mott transition occurs somewhere in this concentration range. The suggestion is supported by the fact that the critical impurity concentration n_c of the Mott transition is calculated from the formula¹⁷ $a_B n_c^{1/3} = 0.25$ to be $1.4 \times 10^{19} \text{ cm}^{-3}$. On the other hand, neither the ps approaches nor the BT approach can explain the rapid increase of μ . This is understood from the fact that the Green's function has been obtained under the ensemble average: No mechanism of the Anderson localization is included. In contrast, the present ps approach is expected to be powerful in the range of $n_i > n_c$ for explaining the experimental data, as shown by one open circle only. At present we have no data available for supporting this view over a sufficiently wide range of $n_i > n_c$. Unfortunately, existing data¹⁷⁻¹⁹ of *n*-type Si and *n*-type Ge at low temperatures are not available for $n_i > n_c$ since the criterion of neither (3.21) nor (3.22) is satisfied. Nevertheless, the present ps results agree qualitatively with the experimental fact that μ is nearly constant for n_i exceeding n_c up to a value by about one order of magnitude larger than n_c , beyond which μ decreases with n_i . It is concluded therefore that the present ps approach offers a powerful tool for analyzing the physical properties of heavily doped semiconductors.

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