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Analysis of ionized-impurity-scattering relaxation time and mobility by the phase-shift method for two interacting valence bands

B. W. Kim* and A. Majerfeld
Department of Electrical and Computer Engineering, Campus Box 425, University of Colorado, Boulder, Colorado 80309

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We present a theoretical method to calculate the phase shifts of the carrier wave function resulting from intraband and interband scattering in the two valence bands of p-type semiconductors. Using the phase-shift method, it is possible to calculate separate ionized-impurity-scattering relaxation times for carriers in the heavy- and light-hole bands and, thereby, obtain a new computation for the mobility of holes in heavily doped materials. Numerical computations of the ionized-impurity-scattering mobility are performed for p-type GaAs over the hole density range $p=10^{17}-10^{20}\,\mathrm{cm}^{-3}$. It is found that the use of the Born approximation results in a small overestimation of the scattering rates at low-carrier densities, but in a significant underestimation for degenerate-carrier densities. For $p>10^{19}\,\mathrm{cm}^{-3}$ the mobility calculated at 300 K by the phase-shift method is approximately 40% lower than the value obtained from the Born approximation.

I. INTRODUCTION

The Born approximation has been used extensively to calculate ionized-impurity-scattering mobilities in semiconductors. Although one obtains simple analytic expressions for the scattering cross section, the Born approximation is only valid in certain limited circumstances.[1] For this reason, the partial-wave phase-shift method has been used as an excellent alternative. On the other hand, the multichannel scattering theory, which is based on the use of wave packets, provides a general formalism to treat scattering problems.[2] However, it is difficult to apply this theory directly to a multiband system, such as the valence bands of semiconductors, as detailed procedures are not available to obtain the phase shifts resulting from interband scattering events. Even though a number of phase-shift treatments for ionized impurity scattering have been reported, the phase-shift method has been developed and applied only to single-band systems.[3-9] As the valence band of semiconductors is made up of heavy- and light-hole bands, there is an intrinsic difficulty in using the single-band phase-shift method for multiband systems because of the change in the effective mass of the scattered particle during an interband scattering event. In order to overcome this difficulty, the heavy- and light-hole bands were combined into an equivalent single band, and the variational technique was used to analyze the hole mobility in p-type materials.[8,9] Although this procedure produces reasonable results, it has the drawback that interband scattering cannot be evaluated explicitly; thus one of the main features of multiband scattering processes is hidden in the analysis.

During the last few years, high-quality heavily doped epitaxial GaAs was developed by different growth techniques employing C for p-type doping,[10,11] and used to improve the high-frequency characteristics of the heterojunction bipolar transistor.[12] Therefore, it is timely to develop the theoretical framework for an improved analysis and computation of the transport properties of holes in heavily doped materials. To this end it becomes necessary to develop detailed procedures to obtain phase shifts of the wave function resulting from both intraband and interband scattering events in a multiband p-type semiconductor.

This paper presents a comprehensive derivation of the phase-shift method to treat an interacting two-band system within the domain of the effective-mass formalism for crystals, which makes it possible to calculate separately the relaxation time for each band. It then becomes possible to calculate the true Hall factor and hole Hall mobility by taking into account the multiband structure of the valence band of semiconductors. This is particularly important for heavily doped semiconductors, as the hole densities are highly degenerate and the Born approximation is not valid. Also, in this case, the ionized-impurity-scattering mechanism dominates over all the other scattering mechanisms. We follow the traditional development[13] of the phase-shift method. We assume that both energy bands are isotropic and parabolic. Finally, in order to compare the method presented in this paper with the Born approximation, we obtain numerical computations of the relaxation times and hole mobilities due to ionized impurity scattering over the range of hole densities $p=10^{17}-10^{20}\,\mathrm{cm}^{-3}$.

II. THEORY

If we consider only one-body interactions, the most general Hamiltonian for an interacting two-band system may be written, in the second quantization representation, as

$$\hat{H}(t)=\int d^3r_1\,\frac{\nabla_1\hat{\psi}_1^{\dagger}(1)\nabla_1\hat{\psi}_1(1)}{2m_1}+\int d^3r_1\,\frac{\nabla_1\hat{\psi}_2^{\dagger}(1)\nabla_1\hat{\psi}_2(1)}{2m_2}+\sum_{i,j=1,2}\int d^3r_2\,\hat{U}_{ij}(2)\,, \tag{1}$$

where we use the four-variable notation, $1=(\mathbf{r}_1,t)$ and $2=(\mathbf{r}_2,t)$, $\hat{\psi}_i$ is the field operator for band i $(i=1,2)$, $\hat{\psi}_i^\dagger$ is the Hermitian conjugate of $\hat{\psi}_i$, and the one-body interaction potential operator $\hat{U}_{ij}(2)[=\hat{U}_{ij}(\mathbf{r}_2)]$ is given by

$$\hat{U}_{ij}(2)=\tfrac{1}{2}\hat{\psi}_i^\dagger(2)U_{ij}(2)\hat{\psi}_j(2)\ . \tag{2}$$

The indices i and j indicate that the scattering potential U_{ij} causes a transition of a particle from an initial band j to a final band i, where band indices $i,j=1,2$ for an interacting two-band system. The corresponding equations of motion can be obtained using[3]

$$\frac{i\partial\hat{\psi}_i(t)}{\partial t}=[\hat{\psi}_i(t),\hat{H}(t)] \tag{3}$$

and the commutation relations for $\hat{\psi}_i^\dagger(t)$ and $\hat{\psi}_i(t)$,[13] and are given, in the first quantization representation, by

$$\begin{aligned} H_{11}|\psi_1\rangle+U_{12}|\psi_2\rangle&=\mathcal{E}|\psi_1\rangle\ ,\\ H_{22}|\psi_2\rangle+U_{21}|\psi_1\rangle&=\mathcal{E}|\psi_2\rangle\ , \end{aligned} \tag{4}$$

where

$$H_{ii}=-\frac{\hbar^2\nabla^2}{2m_i}+U_{ii}\equiv H_{ii}^0+U_{ii}\ , \tag{5}$$

and m_i and $\hbar$ are the effective mass in band i and the Planck constant, respectively. The solutions to Eqs. (4) can be written as

$$|\psi_i\rangle=|\varphi_i\rangle+\frac{1}{\mathcal{E}-H_{ii}^0-U_{ii}}U_{ii'}|\psi_{i'}\rangle\ , \tag{6}$$

where $i\neq i'$ (hereafter we shall use this convention; for example, for band $i=1$, the band index i' designates band 2, and vice versa), and $|\varphi_i\rangle$ is the intraband interaction eigenket of H_{ii}, which satisfies

$$(H_{ii}-\mathcal{E})|\varphi_i\rangle=0\ . \tag{7}$$

The presence of $|\varphi_i\rangle$ in Eq. (6) is reasonable, because $|\psi_i\rangle$ must reduce to $|\varphi_i\rangle$ as the interband scattering potential, $U_{ii'}$, vanishes. The boundary condition for the outgoing wave, which can be chosen, is incorporated by making the energy $\mathcal{E}$ slightly complex[13] in Eq. (6), which in the position representation reads

$$\begin{aligned} \langle\mathbf{r}|\psi_i\rangle=\langle\mathbf{r}|\varphi_i\rangle+\int d^3r'\left\langle\mathbf{r}\left|\frac{1}{\mathcal{E}-H_{ii}^0-U_{ii}+i\eta}\right|\mathbf{r}'\right\rangle\\ \times\langle\mathbf{r}'|U_{ii'}|\psi_{i'}\rangle\ , \end{aligned} \tag{8}$$

with η being an infinitesimal positive constant. Equation (8) may be regarded as the Lippmann-Schwinger (LS) equation for the interacting two-band system. The kernel of this integral equation is the Green's function, which satisfies the equation of motion

$$[H_{ii}^0+U_{ii}(\mathbf{r})-\mathcal{E}]G_i(\mathbf{r},\mathbf{r}')=-\delta(\mathbf{r}-\mathbf{r}')\ . \tag{9}$$

Thus Eq. (8) can be rewritten as

$$\psi_i(\mathbf{r})=\varphi_i(\mathbf{r})+\int d^3r'G_i(\mathbf{r},\mathbf{r}')U_{ii'}(\mathbf{r}')\psi_{i'}(\mathbf{r}')\ . \tag{10}$$

Also, the Green's function in Eq. (9) can be expanded as

$$\begin{aligned} G_i&=\frac{1}{\mathcal{E}-H_{ii}^0-U_{ii}+i\eta}\\ &=\frac{1}{\mathcal{E}-H_{ii}^0+i\eta}+\frac{1}{\mathcal{E}-H_{ii}^0+i\eta}U_{ii}\left[\frac{1}{\mathcal{E}-H_{ii}^0+i\eta}+\frac{1}{\mathcal{E}-H_{ii}^0+i\eta}U_{ii}\frac{1}{\mathcal{E}-H_{ii}^0+i\eta}+\cdots\right]\\ &=G_i^0+G_i^0\Sigma_{ii}^0G_i\ , \end{aligned} \tag{11}$$

where $\Sigma_{ii}^0\equiv U_{ii}$, and the unperturbed Green's function $G_i^0[=G_i^0(\mathbf{r},\mathbf{r}')=G^0(k_i,\mathbf{r},\mathbf{r}')]$ satisfies the equation of motion

$$\left[-\frac{\hbar^2\nabla^2}{2m_i}-\mathcal{E}\right]G_i^0(\mathbf{r},\mathbf{r}')=-\delta(\mathbf{r}-\mathbf{r}')\ . \tag{12}$$

Thus from Eqs. (7) and (12), $\varphi_i(\mathbf{r})$ can be written as

$$\varphi_i(\mathbf{r})=e^{i\mathbf{k}_i\cdot\mathbf{r}}+\int d\mathbf{r}'G_i^0(\mathbf{r}-\mathbf{r}')U_{ii}(\mathbf{r}')\varphi_i(\mathbf{r}')\ . \tag{13}$$

Using Eq. (11), $|\psi_i\rangle$ can be written as

$$\begin{aligned} |\psi_i\rangle&=\sum_{n=0}^{\infty}[G_iU_{ii'}G_{i'}U_{i'i}]^n[|\varphi_i\rangle+G_iU_{ii'}|\varphi_{i'}\rangle]\\ &=\frac{1}{1-G_iU_{ii'}G_{i'}U_{i'i}}[|\varphi_i\rangle+G_iU_{ii'}|\varphi_{i'}\rangle]\ , \end{aligned} \tag{14}$$

where for the second equality we assume that $|G_iU_{ii'}G_{i'}U_{i'i}|<1$, which is a reasonable assumption for a weak scattering potential U_{ij}. For ionized impurity scattering and a dilute impurity concentration, Eq. (14) can be approximated by keeping only terms up to first order in the scattering potential. In this case, Eq. (14) in the position representation reads

$$\begin{aligned} \psi_i(\mathbf{r})&\cong\varphi_i(\mathbf{r})+\int d\mathbf{r}'G_i^0(\mathbf{r}-\mathbf{r}')U_{ii'}(\mathbf{r}')\varphi_{i'}(\mathbf{r}')\\ &=e^{i\mathbf{k}_i\cdot\mathbf{r}}+\int d\mathbf{r}'G_i^0(\mathbf{r}-\mathbf{r}')U_{ii}(\mathbf{r}')\varphi_i(\mathbf{r}')\\ &\quad+\int d\mathbf{r}'G_i^0(\mathbf{r}-\mathbf{r}')U_{ii'}(\mathbf{r}')\varphi_{i'}(\mathbf{r}')\ . \end{aligned} \tag{15}$$

The unperturbed Green's function G_i^0 and its asymptotic form at large distance are given, respectively, by

$$\begin{aligned} &G_i^0(\mathbf{r}-\mathbf{r}')\\ &\quad=-\frac{m_i}{2\pi\hbar^2}\frac{e^{i\mathbf{k}_i|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}\xrightarrow[r\to\infty]{}-\frac{m_i}{2\pi\hbar^2}\frac{e^{i\mathbf{k}_i\mathbf{r}}}{r}e^{i\mathbf{k}_i'\cdot\mathbf{r}'}\ , \end{aligned} \tag{16}$$

where $\mathbf{k}_i' = \hat{r} k_i$. Thus, by substituting Eq. (16) into Eq. (15), the asymptotic form of the scattered wave function at large distance is obtained as

$$\psi_i(\mathbf{r}) \xrightarrow[r\to\infty]{} \frac{1}{(2\pi)^{3/2}} \left[e^{i\mathbf{k}_i\cdot\mathbf{r}} + f_{ii}\frac{e^{i\mathbf{k}_i\mathbf{r}}}{r} + f_{ii'}\frac{e^{i\mathbf{k}_i\mathbf{r}}}{r} \right] , \tag{17}$$

where the normalization constant $1/(2\pi)^{3/2}$ is introduced and the scattering amplitude f_{ij} is defined as[14]

$$\begin{aligned}
f_{ij} &\equiv f(\mathbf{k}_i', \mathbf{k}_j) \\
&= -\frac{1}{4\pi}\frac{2m_i}{\hbar^2}(2\pi)^3 \int d\mathbf{r}' \frac{e^{-i\mathbf{k}_i'\mathbf{r}'}}{(2\pi)^{3/2}} U_{ij}(\mathbf{r}')\langle \mathbf{r}' | \varphi_j \rangle \\
&= -\frac{1}{4\pi}\frac{2m_i}{\hbar^2}(2\pi)^3 \langle \mathbf{k}_i' | U_{ij} | \varphi_j \rangle \\
&= -\frac{1}{4\pi}\frac{2m_i}{\hbar^2}(2\pi)^3 \langle \mathbf{k}_i' | T_{ij} | \mathbf{k}_j \rangle \\
&= -\frac{4\pi^2 m_i}{\hbar^2} \sum_{l_i, m_i, l_j, m_j} \int d\mathscr{E}_i \int d\mathscr{E}_j \langle \mathbf{k}_i' | \mathscr{E}_i, l_i, m_i \rangle \langle \mathscr{E}_i, l_i, m_i | T_{ij} | \mathscr{E}_j, l_j, m_j \rangle \langle \mathscr{E}_j, l_j, m_j | \mathbf{k}_j \rangle \\
&= -\frac{4\pi^2 m_i}{\hbar^2} \sum_{l_i, m_i, l_j, m_j} \int d\mathscr{E}_i \int d\mathscr{E}_j \frac{\hbar}{\sqrt{m_i k_i}} \delta \left[\mathscr{E}_i - \frac{\hbar^2 k_i^2}{2m_i} \right] Y_{l_i}^{m_i}(\hat{k}_i') T_{ij}^{l_i}(\mathscr{E}_i) \delta_{l_i l_j} \delta_{m_i m_j} \frac{\hbar}{\sqrt{m_j k_j}} \delta \left[\mathscr{E}_j - \frac{\hbar^2 k_j^2}{2m_j} \right] Y_{l_j}^{m_j}(\hat{k}_j)^* \\
&= -\frac{4\pi^2 m_i}{\hbar^2} \sum_{l_i, m_i} \frac{\hbar}{\sqrt{m_i k_i}} \frac{\hbar}{\sqrt{m_j k_j}} T_{ij}^{l_i}(\mathscr{E}_i) \delta(\mathscr{E}_i - \mathscr{E}_j) Y_{l_i}^{m_i}(\hat{k}_i') Y_{l_i}^{m_i}(\hat{k}_j) ,
\end{aligned} \tag{18}$$

where $Y_{l_i}^{m_i}(\hat{k}_i')$ is the angular part of the wave function $\varphi_i(\mathbf{r})$ associated with the direction along $\hat{k}_i'$ with the orbital and magnetic angular momentum l_i and m_i, respectively, $\mathscr{E}_i$ $[\equiv \mathscr{E}(k_i)]$ and $\mathscr{E}_j$ $[\equiv \mathscr{E}(k_j)]$ are the energies of particles in band i and band j, respectively, and the transition matrix $T_{\mathbf{k}_i'\mathbf{k}_j}$ for the transition from the state $|\mathbf{k}_j\rangle$ of band j to the state $|\mathbf{k}_i'\rangle$ of band i is introduced:

$$\begin{aligned}
T_{\mathbf{k}_i'\mathbf{k}_j} &= (2\pi)^3 \langle \mathbf{k}_i' | T_{ij} | \mathbf{k}_j \rangle \\
&= (2\pi)^3 \langle \mathbf{k}_i' | U_{ij} | \varphi_j \rangle = -\frac{2\pi\hbar^2}{m_i} f(\mathbf{k}_i', \mathbf{k}_j) ,
\end{aligned} \tag{19}$$

and use was made of the equalities

$$\langle \mathbf{k} | \mathscr{E}, l, m \rangle = \frac{\hbar}{\sqrt{mk}} \delta \left[\mathscr{E} - \frac{\hbar^2 k^2}{2m} \right] Y_l^m(\hat{k}) , \tag{20}$$

$$\langle \mathscr{E}_i, l_i, m_i | T_{ij} | \mathscr{E}_j, l_j, m_j \rangle = T_{ij}^{l_i}(\mathscr{E}_i) \delta_{l_i l_j} \delta_{m_i m_j} . \tag{21}$$

It should be noted that if we replace φ_j by $e^{i\mathbf{k}_j\cdot\mathbf{r}}$ in Eq. (18), we than obtain the scattering amplitude in the Born approximation. To obtain the angular dependence of the scattering amplitude, we choose the coordinate system in such a way that the wave vector of the initial states $(\mathbf{k}_j; j=1,2)$ is in the positive-z direction as shown in Fig. 1, which leads to

$$\begin{aligned}
Y_l^m(\hat{k}_j) &= \left[\frac{2l+1}{4\pi} \right]^{1/2} \delta_{m0} , \\
Y_l^0(\hat{k}_i') &= \left[\frac{2l+1}{4\pi} \right]^{1/2} P_l(\cos\theta) ,
\end{aligned} \tag{22}$$

where P_l is the Legendre polynomial of order l, and θ is the angle between $\mathbf{k}_i'$ and $\mathbf{k}_j$. Thus, using Eqs. (22), Eq. (18) can be simplified to be

$$f_{ij} = \sum_l (2l+1) f_{ij}^l(k_i, k_j; \mathscr{E}_i) P_l(\cos\theta) , \tag{23}$$

where

$$\begin{aligned}
&f_{ij}^l(k_i, k_j; \mathscr{E}_i) \\
&\qquad = -\left[\frac{m_i}{m_j} \right]^{1/2} \frac{\pi}{\sqrt{k_i k_j}} T_{ij}^l(\mathscr{E}_i) \delta(\mathscr{E}_i - \mathscr{E}_i) .
\end{aligned} \tag{24}$$

Using Eq. (23), the scattered wave function of Eq. (17) at large distance can be written as

$$\psi_i(\mathbf{r}) \xrightarrow[r\to\infty]{} \frac{1}{(2\pi)^{3/2}} \sum_l (2l+1) P_l(\cos\theta) \left\{ \frac{e^{i\mathbf{k}_i\mathbf{r}} - e^{-i(\mathbf{k}_i\mathbf{r} - l\pi)}}{2ik_i r} + [f_{ii}^l(k_i, k_i; \mathscr{E}) + f_{ii'}^l(k_i, k_{i'}; \mathscr{E})] \frac{e^{ik_i r}}{r} \right\} , \tag{25}$$

where we used

$$e^{ikz} = \sum_{l=0}^{\infty} i^l (2l+1) P_l(\cos\theta) j_l(kr) \xrightarrow[r\to\infty]{} \sum_{l=0}^{\infty} (2l+1) P_l(\cos\theta) \frac{e^{ikr} - e^{-i(kr - l\pi)}}{2ikr} . \tag{26}$$

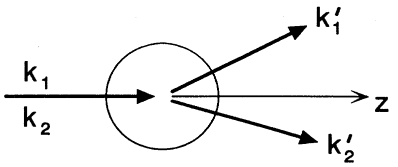


FIG. 1. Direction of incoming ($\mathbf{k}_1$ and $\mathbf{k}_2$) and outgoing waves ($\mathbf{k}_1'$ and $\mathbf{k}_2'$) waves after a scattering event.

In order to insure conservation of flux during elastic scattering (incoming flux must be equal to outcoming flux for elastic scattering), we introduce the scattering matrix S which satisfies

$$S_i^l = 1 + 2ik_i[f_{ii}^l(k_i,k_i;\mathscr{E}) + f_{ii'}^l(k_i,k_{i'};\mathscr{E})]$$
$$\equiv e^{2i\delta_i^l(\mathscr{E})} \ . \tag{27}$$

Thus, on substituting Eq. (27) into Eq. (25), the radial part of $\psi_i(\mathbf{r})$ with orbital angular momentum l, $\overline{R}_i^l(\mathbf{r})$, at large distance takes the form

$$\overline{R}_i^l(\mathbf{r}) \xrightarrow[r\to\infty]{} \frac{C_l(k_i,k_{i'})}{k_i r} \sin[k_i r + \delta_i^l(k_i,k_{i'}) - l\pi/2] \ , \tag{28}$$

in which $C_l(k_i,k_{i'})$ is a normalization constant. From Eqs. (25) and (27), it can easily be shown that flux is conserved.

In order to decompose δ_i^l into δ_{ii}^l (intraband phase shift) and $\delta_{ii'}^l$ (interband phase shift), and to evaluate these, we start by expanding, respectively, the plane wave $\varphi_i(\mathbf{r})$, and the unperturbed Green's function in the outgoing wave boundary condition:[13]

$$e^{i\mathbf{k}_i\cdot\mathbf{r}} = \sum_l (2l+1) i^l P_l(\hat{\mathbf{k}}_i\cdot\hat{\mathbf{r}}) j_l(k_i r) \ , \tag{29}$$

$$\varphi_i(\mathbf{r}) = \sum_l (2l+1) i^l P_l(\hat{\mathbf{k}}_i\cdot\hat{\mathbf{r}}) R_i^l(k_i r) \ , \tag{30}$$

$$G^0(k_i,\mathbf{r}-\mathbf{r}') = \pi\rho(k_i) \sum_l (2l+1) P_l(\hat{\mathbf{r}}\cdot\hat{\mathbf{r}}')$$
$$\times [j_l(k_i r_<)\eta_l(k_i r_>) - i j_l(k_i r_<) j_l(k_i r_>)] \ , \tag{31}$$

where j_l and η_l are the spherical Bessel functions of the first and second kinds, respectively, of order l, $h_l^\dagger = -\eta_l + i j_l$, $\rho(k_i) = k_i m_i / 2(\hbar\pi)^2$ is the density of states in band i, and $r_<$ and $r_>$ respectively, denote the smaller and the larger of the two lengths r and r'. Here the radial function of $\varphi_i(\mathbf{r})$, $R_i^l(k_i r)$, satisfies the equation

$$\left\{ -\frac{\hbar^2}{2m_i} \left[\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} - \frac{l(l+1)}{r^2} \right] + [U_{ii}(\mathbf{r}) - \mathscr{E}(k_i)] \right\} R_i^l(k_i r) = 0 \ . \tag{32}$$

On substituting Eqs. (29)–(31) into Eq. (15), $\overline{R}_i^l(k_i r)$ is given by

$$\overline{R}_i^l(k_i r) = j_l(k_i r) + 4\pi^2\rho(k_i) \int_0^\infty r'^2 dr' j_l(k_i r_<) h_l^\dagger(k_i r_>) U_{ii}(r') R_i^l(k_i r')$$
$$+ 4\pi^2\rho(k_i) \int_0^\infty r'^2 dr' j_l(k_i r_<) h_l^\dagger(k_i r_>) U_{ii'}(r') R_{i'}^l(k_{i'} r') \ . \tag{33}$$

In the asymptotic limit at large distance, this integral equation can be written as

$$\overline{R}_i^l(k_i r) \xrightarrow[r\to\infty]{} j_l(k_i r) + [D_{ii}^l(k_i)\eta_l(k_i r) + D_{ii'}^l(k_i)\eta_l(k_i r)] - i[D_{ii}^l(k_i) j_l(k_i r) + D_{ii'}^l(k_i) j_l(k_i r)]$$
$$\xrightarrow[r\to\infty]{} \frac{\sin(k_i r - l\pi/2)}{k_i r} - (D_{ii}^l + D_{ii'}^l)\frac{\cos(k_i r - l\pi/2)}{k_i r} - i(D_{ii}^l + D_{ii'}^l)\frac{\sin(k_i r - l\pi/2)}{k_i r} \ , \tag{34}$$

where

$$D_{ij}^l = 4\pi^2\rho(k_i) \int_0^\infty r^2 dr\, j_l(k_i r) U_{ij}(r) R_j^l(k_j r) \ , \tag{35}$$

and $\hbar^2 k_i^2/2m_i = \hbar^2 k_j^2/2m_j$, which assures energy conservation, as required for elastic scattering; hereafter, this is implicitly assumed. The potential $U_{ij}(r)$ is assumed to be of short range, i.e., it falls off faster than $1/r^2$ at large distances. This is necessary for the integral in Eq. (35) to be well defined.

As the two asymptotic expressions of Eqs. (28) and (34) must be identical, we set

$$D_{ii}^l + D_{ii'}^l = -\exp(i\delta_i^l)\sin(\delta_i^l) \ . \tag{36}$$

Thus the proper choice of normalization constant is

$$C_l(k_i,k_{i'}) = \exp[i\delta_i^l(k_i,k_{i'})] \ . \tag{37}$$

The phase shift given in Eq. (36) can be separated by setting

$$D_{ii}^l = -\frac{\exp[2i(\delta_{ii}^l + \zeta)] - 1}{2i} \ ,$$
$$D_{ii'}^l = -\exp[2i(\delta_{ii}^l + \zeta)]\frac{\exp[2i(\delta_{ii'}^l - \zeta)] - 1}{2i} \tag{38}$$

where

$$\delta_i^l = (\delta_{ii}^l + \zeta) + (\delta_{ii'} - \zeta) \ , \tag{39}$$

and ζ represents an arbitrariness in the choice of phase. Finally, combining Eqs. (35) and (38), we obtain

$$D_{ii}^l = -e^{i\delta_{ii}^l}\sin(\delta_{ii}^l)$$
$$= 4\pi^2\rho(k_i) \int_0^\infty r^2 dr\, j_l(k_i r) U_{ii}(r) R_i^l(k_i r) \ , \tag{40}$$

$$\begin{aligned}D^l_{ii'}&=-e^{i2\delta^l_{ii}}e^{i\delta^l_{ii'}}\sin(\delta^l_{ii'})\\&=4\pi^4\rho(k_i)\int_0^\infty r^2dr\, j_l(k_ir)U_{ii'}(r)R^l_{i'}(k_{i'}r)\ ,\end{aligned}\tag{41}$$

where we set $\zeta=0$ as D^l_{ii}, and $D^l_{ii'}$ must vanish when $U_{ii}(r)=U_{ii'}(r)=0$. From Eqs. (18), (19), and (35), the relation between the transition matrix, the scattering amplitude, and D^l_{ij} can be established as

$$\begin{aligned}T_{\mathbf{k}'_i\mathbf{k}_j}&=-\frac{2\pi\hbar^2}{m_i}f(\mathbf{k}'_i,\mathbf{k}_j)\\&=\frac{2\pi\hbar^2}{m_ik_i}\sum_l(2l+1)P_l(\cos\theta)D^l_{ij}\ .\end{aligned}\tag{42}$$

The procedure to determine phase shifts for the interacting two-band system is as follows: The radial wave functions for intraband interactions, $R^l_i(k_ir)$, are solved first from Eq. (32). Then from Eq. (40) the intraband phase shift δ^l_{ii} is determined. Finally, the interband phase shift $\delta^l_{ii'}$ is obtained from Eq. (41) once δ^l_{ii} is known.

In order to obtain the differential scattering cross section $d\sigma/d\Omega$, where Ω is the solid angle, consider a large number of identically prepared particles. The differential cross section for intraband and interband transitions can be defined, respectively, as

$$\frac{d\sigma_{ii}}{d\Omega}d\Omega=\frac{\begin{array}{c}\text{number of particles scattered into } d\Omega\\ \text{per unit time from band } i \text{ to band } i\end{array}}{\begin{array}{c}\text{number of incident particles through}\\ \text{band } i \text{ crossing unit area per unit time}\end{array}}=\frac{r^2|j^{\text{sc}}_{i\to i}|}{|j^{\text{in}}_i|}=|f(\mathbf{k}'_i,\mathbf{k}_i)|^2d\Omega\ ,\tag{43}$$

$$\frac{d\sigma_{ii'}}{d\Omega}d\Omega=\frac{\begin{array}{c}\text{number of particles scattered into } d\Omega\\ \text{per unit time from band } i' \text{to band } i\end{array}}{\begin{array}{c}\text{number of incident particles through}\\ \text{band } i'\text{crossing unit area per unit time}\end{array}}=\frac{k_im_{i'}}{k_{i'}m_i}\frac{r^2|j^{\text{sc}}_{i'\to i}|}{|j^{\text{in}}_{i'}|}=\frac{k_im_{i'}}{k_{i'}m_i}|f(\mathbf{k}'_i,\mathbf{k}_{i'})|^2d\Omega\ .\tag{44}$$

Therefore, using Eqs. (40)–(42), the total cross sections for intraband and interband transitions are given, respectively, by

$$\sigma^{\text{tot}}_{ii}=\int|f(\mathbf{k}'_i,\mathbf{k}_i)|^2\left\{\begin{array}{c}1\\1-\cos\theta\end{array}\right\}d\Omega=\frac{4\pi}{k_i^2}\sum_l\left\{\begin{array}{c}(2l+1)\sin^2(\delta^l_{ii})\\(l+1)\sin^2(\delta^l_{ii}-\delta^{l+1}_{ii})\end{array}\right\}\ ,\tag{45}$$

$$\sigma^{\text{tot}}_{ii'}=\frac{k_im_{i'}}{k_{i'}m_i}\int|f(\mathbf{k}'_i,\mathbf{k}_{i'})|^2\left\{\begin{array}{c}1\\1-\cos\theta\end{array}\right\}d\Omega=\frac{m_{i'}}{m_i}\frac{4\pi}{k_ik_{i'}}\sum_l\left\{\begin{array}{c}(2l+1)\sin^2(\delta^l_{ii'})\\(l+1)\sin^2(\delta^l_{ii'}-\delta^{l+1}_{ii'})\end{array}\right\}\ .\tag{46}$$

On the other hand, the presence of two interacting bands of carriers introduces considerable complexity into transport calculations. The standard way of handling this problem, within the semiclassical regime, is to first set up the Boltzmann equations for the two-band system, and then solve the resultant coupled equations. The derivation and the exact solution to first order in the external electric field **E**, in the isotropic band approximation, are shown in the Appendix. The quantities q_{ij}'s, which correspond in their characteristics to the inverse of the relaxation time, can be calculated according to Eqs. (A8):

$$\begin{aligned}q_{ii}&=\frac{2\pi}{\hbar}\frac{n_I}{(2\pi)^3}\pi\left[\frac{2m'_i}{\hbar^2}\right]^{3/2}\int\cos\theta\,d\theta\int\sqrt{\mathcal{E}'_i}\,d\mathcal{E}'_i\delta(\mathcal{E}'_i-\mathcal{E}_i)|T_{ii}|^2(1-\cos\theta)\\&=\left[\frac{2}{m'_i}\right]^{3/2}\frac{\pi\hbar^2n_I}{\sqrt{\mathcal{E}'_i}}\sum_l(l+1)\sin^2(\delta^l_{ii}-\delta^{l+1}_{ii})\ ,\\q_{i'i}&=\frac{2\pi}{\hbar}\frac{n_I}{(2\pi)^3}\pi\left[\frac{2m'_i}{\hbar^2}\right]^{3/2}\int\cos\theta\,d\theta\int\sqrt{\mathcal{E}'_i}\,d\mathcal{E}'_i\delta(\mathcal{E}'_i-\mathcal{E}_{i'})|T_{ii'}|^2\\&=\left[\frac{2}{m'_i}\right]^{3/2}\frac{\pi\hbar^2n_I}{\sqrt{\mathcal{E}'_i}}\sum_l(2l+1)\sin^2(\delta^l_{ii'})\ ,\\q'_{i'i}&=-\frac{2\pi}{\hbar}\frac{n_I}{(2\pi)^3}\pi\left[\frac{2m'_i}{\hbar^2}\right]^{3/2}\int\cos\theta\,d\theta\int\sqrt{\mathcal{E}'_i}\,d\mathcal{E}'_i|T_{ii'}|^2\left[\frac{m'_{i'}}{m_i}\right]^{1/2}\cos\theta\\&=-\left[\frac{2}{m'_i}\right]^{3/2}\frac{\pi\hbar^2n_I}{\sqrt{\mathcal{E}'_i}}\left[\frac{m'_{i'}}{m_i}\right]^{1/2}\sum_l2(l+1)\sin(\delta^l_{ii'})\sin(\delta^{l+1}_{ii'})\cos(\delta^l_{ii'}-\delta^{l+1}_{ii'})\ ,\end{aligned}\tag{47}$$

where n_I is the density of ionized impurities, m (m') and $\mathcal{E}$ ($\mathcal{E}'$), respectively, designate the effective mass and energy of a carrier in the initial (final) band, and the first and second indices of the inverse relaxation times ($q_{ii}, q_{i'i}, q'_{i'i}$) designate the initial and final bands, respectively, involved in a scattering event; q_{ii} gives the transition probability weighted with $(1-\cos\theta)$ due to intraband scattering, and $q_{i'i}$ and $q'_{i'i}$ describe transition probabilities weighted with 1 and $\cos\theta$, respectively, due to interband scattering. In Eqs. (47) we used the relation between the differential scattering rate S_{ij} and the transition matrix for ionized impurity scattering:

$$S_{ij}=\frac{2\pi}{\hbar}\frac{n_I}{(2\pi)^3}|T_{ji}|^2 . \tag{48}$$

III. NUMERICAL RESULTS

The scattering of holes in the heavy- and light-hole bands of p-type GaAs by ionized impurities is calculated by the phase-shift method developed in Sec. II and, also, in the Born approximation over the hole density range $1\times10^{17}-1\times10^{20}$ cm^{-3}. The Born approximation is valid when carrier energies are high relative to the interaction potential, but is invalid for carriers with energies near band extrema, as in this case the carriers are strongly scattered by the screened Coulomb potential. The phase-shift method, based on a maximum of 50 partial waves, gives more accurate results because it is valid for all carrier energies.

The corresponding inverse relaxation times in the Born approximation can be calculated according to Eqs. (A8), and are given by

$$\begin{aligned} q_{ii}&=\frac{n_Ie^4}{64\sqrt{2}\pi\varepsilon^2\sqrt{m_i}(k_BT)^{3/2}}\frac{1}{K^{3/2}}\\ &\quad\times\left[(3A-1)^2\ln\frac{|A+1|}{|A-1|}-2\left[9A-6+\frac{4}{A+1}\right]\right] ,\\ q_{ii'}&=\frac{3n_Ie^4\sqrt{m_{i'}}}{64\sqrt{2}\pi\varepsilon^2m_i(k_BT)^{3/2}}\frac{1}{K^{3/2}}\left[2A\ln\frac{|A+1|}{|A-1|}-4\right] ,\\ q'_{ii'}&=-\frac{3n_Ie^4}{64\sqrt{2}\pi\varepsilon^2\sqrt{m_i}(k_BT)^{3/2}}\frac{1}{K^{3/2}}\\ &\quad\times\left[6A+(3A^2-1)\ln\frac{|A-1|}{|A+1|}\right] , \end{aligned} \tag{49}$$

where e, k_B, and ε respectively, are the electron charge, the Boltzmann constant, and the dielectric constant, and

$$A=\frac{M+1+Q/K}{2\sqrt{M}},\quad K=\frac{\hbar^2k_i^2}{2m_ik_BT},\quad Q=\frac{\hbar^2q_s^2}{2m_ik_BT} . \tag{50}$$

Here $M=1$ for q'_{ii} and $M=m'/m$ for both $q_{i'i}$ and $q'_{i'i}$, and q_s is the inverse screening length given by

$$q_s^2=\frac{e^2p}{2\varepsilon k_BT}\frac{F_{-1/2}}{F_{+1/2}} , \tag{51}$$

with the total carrier concentration of p ($p=p_1+p_2$; p_1 and p_2 are the hole densities in bands 1 and 2, respectively) and F_r for the Fermi integral of order r:

$$\begin{aligned} &F_r(\eta_F)=\int_0^\infty\frac{x^rdx}{1+e^{x-\eta_F}},\quad \eta_F=\frac{\mathcal{E}_F}{k_BT} ,\\ &\mathcal{E}_F=\text{Fermi energy} . \end{aligned} \tag{52}$$

We used the Thomas-Fermi screening, rather than other more sophisticated methods, as it should give a reasonable numerical result, in view of the complexity of the valence band. The overlap functions,[15] which represent the anisotropy of scattering due to the symmetry properties of the wave functions of Bloch holes, are taken into account in the above equations.

The upper bound in the phase-shift sum was determined by the criterion that the next term in the series should be less than 1% of the leading term. The upper limit of 50 partial waves satisfied the desired numerical accuracy over the hole concentration range considered in this work. The Schrödinger equation was solved by the Numerov method,[16] and the end point of the screened Coulomb potential was selected when it dropped below 0.1% of the value of the potential at the screening length. Once the relaxation times were determined using Eq. (A7), the mobility for holes in band i were calculated by

$$\mu_i=e\langle\tau_i(\mathcal{E})\rangle/m_i , \tag{53}$$

where $\langle\ \rangle$ denotes an average over carrier energies (the

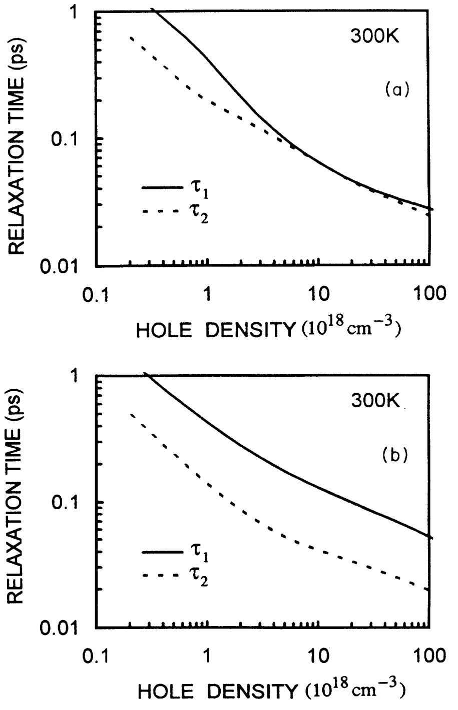
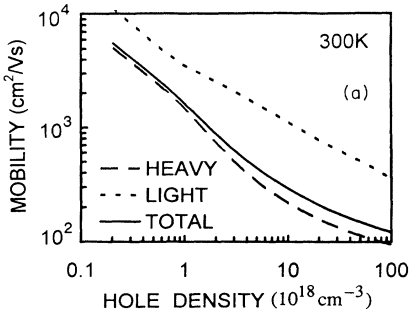


FIG. 2. Momentum relaxation times due to ionized impurity scattering, calculated at 300 K using (a) the phase-shift method, and (b) the Born approximation, where τ_1 and τ_2 correspond to the heavy and light holes, respectively.



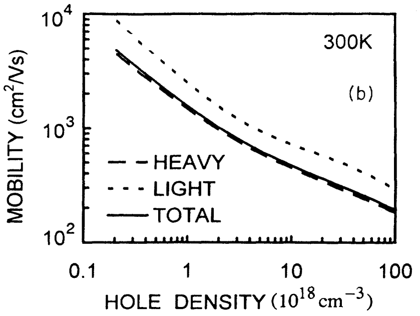


FIG. 3. Ionized impurity scattering mobilities for heavy and light holes, and total mobility, calculated at 300 K using (a) the phase-shift method and (b) the Born approximation.

upper limit for this integration was $10k_BT$ above the Fermi energy, or $10k_BT$ into the band). The combined two-band hole mobility was obtained from

$$\mu=(p_1\mu_1+p_2\mu_2)/(p_1+p_2) \ . \tag{54}$$

The parameters for the heavy-hole mass, light-hole mass, and dielectric constant used in this calculation were $m_h=0.5m_0$, $m_l=0.088m_0$, and $\varepsilon=12.9$, respectively, where m_0 is the free-electron mass. The numerical results at 300 K are displayed in Fig. 2. The corresponding hole mobilities are presented in Fig. 3.

IV. DISCUSSION AND CONCLUSIONS

It has been several decades since the phase-shift method was first applied to study the scattering of free carriers in a semiconductor by a screened Coulomb potential. The phase-shift method is clearly preferable to the Born approximation as it yields more accurate scattering cross sections. However, it has only been applied to the calculation of impurity scattering in multiband semiconductors by treating the two bands as a single equivalent band and, thereby, not allowing for different cross sections for the intraband and interband scattering processes.

In this paper we developed a method to calculate phase shifts of the carrier wave function resulting from both interband and intraband scattering in the two valence bands of p-type semiconductors. We started with the most general Hamiltonian for the interacting two-band system and derived a generalized Lippmann-Schwinger equation. Then we followed the standard procedure to obtain the phase shifts, i.e., by expanding the LS equation, keeping only terms up to first order in the scattering potential, and by taking the asymptotic limit of the scattered carrier wave functions at a large distance. By this method we determined the phase shifts for both intraband and interband scattering events.

Our results show that the momentum relaxation times obtained for heavy holes at high-carrier densities by the phase-shift method are significantly shorter, by about a factor of 2, than the values obtained by the Born approximation. Also, the relaxation times for light holes are slightly longer for the phase-shift method in comparison to the Born approximation. In summary, the Born approximation overestimates the overall ionized impurity scattering rates for hole concentrations less than 1×10^{18} cm^{-3} and underestimates the rates by approximately 40% for concentrations above 1×10^{19} cm^{-3} This becomes clearly apparent when the data from Figs. 3(a) and 3(b) are combined as in Fig. 4. It should be noted that this appears to be a typical and, possibly, a general result of the Born approximation, as it was previously note by Lowney and Bennett[8] from a variational calculation using an effective single band for p-type GaAs and by Meyer and Bartoli[1] for p-type Si.

It is appropriate to mention that the results of Fig. 4 should not be compared directly with experimental mobilities, as a detailed mobility calculation should include a number of additional scattering mechanisms for hole densities not highly degenerate. Comprehensive mobility and Hall factor calculations for p-type GaAs at room temperature, using the phase-shift method for ionized impurity scattering presented here, will be published elsewhere. Finally, it should be noted that in the past a value of unity for the Hall factor has generally been assumed, which leads to an incorrect determination of mobility and hole density from experimental Hall effect data. We conclude that it is important to calculate relaxation times separately for each hole band in p-type materials, especially for highly degenerate carrier densities, as the ionized impurity scattering mechanism dominates over all other scattering mechanisms.

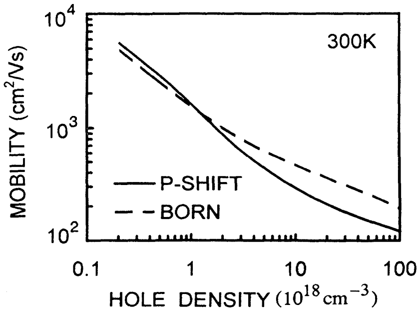


FIG. 4. Comparison of ionized-impurity-scattering mobilities as calculated at 300 K using the phase-shift method and the Born approximation.

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APPENDIX

The scattering processes centered at band i ($i=1$ and 2) can be expressed as

$$\begin{aligned} S_i &= S(\mathbf{k}_i,\mathbf{k}_i')+S(\mathbf{k}_i,\mathbf{k}_{i'}')\equiv S_{ii}+S_{ii'}\ , \\ S_i' &= S(\mathbf{k}_i',\mathbf{k}_i)+S(\mathbf{k}_{i'}',\mathbf{k}_i)\equiv S_{ii}'+S_{i'i}'\ , \end{aligned} \tag{A1}$$

where $i\neq i'$, $S(\mathbf{k}_i,\mathbf{k}_j')$ is the differential scattering rate for a transition from an initial state $\mathbf{k}$ in band i to a final state $\mathbf{k}'$ in band j (outgoing scattering), and $S(\mathbf{k}_j',\mathbf{k}_i)$ is that from state $\mathbf{k}'$ in band j to state $\mathbf{k}$ in band i (incoming scattering).

Using the scattering rates defined in Eqs. (A1), a pair of Boltzmann equations can be written as

$$\begin{aligned} \frac{e}{\hbar}E\frac{\partial f_i}{\partial k_i}x_i = \int d\mathbf{k}'[&S_{ii}'(f_i'+x_i\chi_{ii}g_i')(1-f_i-x_ig_i)+S_{i'i}'(f_{i'}'+x_i\chi_{ii'}g_{i'}')(1-f_i-x_ig_i) \\ &-S_{ii}(f_i+x_ig_i)(1-f_i'-x_i\chi_{ii}g_i')-S_{ii'}(f_i+x_ig_i)(1-f_{i'}'-x_i\chi_{ii'}g_{i'}')]\ , \end{aligned} \tag{A2}$$

in the isotropic band approximation, where χ_{ij} ($i,j=1,2$) is the cosine of the angle between either $\mathbf{k}_i$ and $\mathbf{k}_j'$ or $\mathbf{k}_i'$ and $\mathbf{k}_j$; g and g' are the perturbation part of the nonequilibrium function $\bar{f}(k_i)$ to first order in $E(=|\mathbf{E}|)$; x_i (x_i') is the cosine of the angle between the electric field $\mathbf{E}$ and $\mathbf{k}_i$ ($\mathbf{k}_i'$), $f_i\equiv f(k_i)$; $f_i'=f(k_i')$; f is the equilibrium Fermi distribution function, and we use the fact $\int x'S(\chi)d\mathbf{k}'=x\int \chi S(\chi)d\mathbf{k}'$ as S is independent of the azimuthal angle. In this approximation, the differential scattering rate can be expressed in terms of $|\mathbf{k}_i|$, $|\mathbf{k}_j'|$ and χ_{ij}, and g and g' depend on wave-vector magnitude; i.e., $g_i=g_i(k)$ and $g_i'=g_i(k')$. In Eq. (A2), we retain only the first two terms in the perturbation expansion of $\bar{f}(k_i)$ under a weak external electric field $\mathbf{E}$, i.e.,

$$\bar{f}(k_i)\cong f_i+x_ig_i \quad\text{and}\quad \bar{f}(k_i')\cong f_i'+x_i'g_i'\ . \tag{A3}$$

As in the isotropic band approximation, all the functions included in Eq. (A2) can be expressed in terms of energy; hereafter we replace the wave vectors by particle energies for those functions. With this replacement, g and g' can be assumed to take the following form for elastic scattering:

$$\begin{aligned} g_i &\equiv g(\mathscr{E}_i)=-\frac{eE\tau(\mathscr{E}_i)}{\hbar}\frac{\partial f(\mathscr{E}_i)}{\partial k_i}\ , \\ g_i' &\equiv g(\mathscr{E}_1')=-\frac{eE\tau(\mathscr{E}_i')}{\hbar}\frac{\partial f(\mathscr{E}_i')}{\partial k_i'}=\left[\frac{m_i'}{m_i}\right]^{1/2}g_i\ , \end{aligned} \tag{A4}$$

where $\mathscr{E}_i$ ($\mathscr{E}_i'$) and m_i (m_i'), respectively, are the energy and effective mass for the initial (final) band i. We note that even though the valence band is not isotropic, except near the band maxima, we take this form of Eqs. (A4) to be valid up to the highest hole density considered in this paper.

Integrating Eq. (A2) over x_1 and x_2, respectively, gives the detailed balance equation

$$S_{ij}'f_i'=S_{ji}f_j\frac{1-f_i'}{1-f_j}\ , \tag{A5}$$

where we make the physically reasonable assumption that the intraband and interband scattering rates separately obey the detailed balance condition.

On the other hand, integrating Eq. (A2) over x_1 and x_2 of the resultant equations multiplied by x_1 and x_2, respectively, gives

$$\begin{aligned} -\frac{e}{\hbar}E\frac{\partial f_i}{\partial k_i}=\pi\left[\frac{2m'}{\hbar^2}\right]^{3/2}\int \cos\theta\, d\theta\int\sqrt{\mathscr{E}'}d\mathscr{E}'\{&S_{ii}'[f_i'g_i-\chi_{ii}(1-f_i)g_i']+S_{i'i}'[f_{i'}'g_i-\chi_{ii'}(1-f_i)g_{i'}'] \\ &+S_{ii}[(1-f_i')g_i-\chi_{ii}f_ig_i']+S_{ii'}[(1-f_{i'}')g_i-\chi_{ii'}f_ig_{i'}']\}\ . \end{aligned} \tag{A6}$$

Replacing g' by g and S' by S in Eq. (A6) using the second equation of Eq. (A4) and Eq. (A5), and solving for g_1 and g_2, we obtain for elastic scattering the solution which is exact to first order in the electric field E:

$$\tau_i=\frac{q_{i'i'}+q_{i'i}-q_{ii'}'}{(q_{ii}+q_{ii'})(q_{i'i'}+q_{i'i})-q_{ii'}'q_{i'i}'}\ , \tag{A7}$$

where

$$\begin{aligned}
q_{ii} &= \pi \left[\frac{2m_i'}{\hbar^2} \right]^{3/2} \int \cos\theta \, d\theta \int \sqrt{\mathcal{E}_i'} d\mathcal{E}_i' S_{ii} \frac{(1-f_i')}{(1-f_i)} \left[1 - \left[\frac{\mathcal{E}_i' m_i}{\mathcal{E}_i m_i'} \right]^{1/2} \cos\theta \right] \delta(\mathcal{E}_i' - \mathcal{E}_i) \, , \\
q_{ii'} &= \pi \left[\frac{2m_{i'}'}{\hbar^2} \right]^{3/2} \int \cos\theta \, d\theta \int \sqrt{\mathcal{E}_i'} d\mathcal{E}_{i'}' S_{ii'} \frac{(1-f_{i'}')}{(1-f_i)} \delta(\mathcal{E}_{i'}' - \mathcal{E}_i) \, , \\
q_{ii'}' &= -\pi \left[\frac{2m_{i'}'}{\hbar^2} \right]^{3/2} \int \cos^2\theta \, d\theta \int \sqrt{\mathcal{E}_{i'}'} d\mathcal{E}_{i'}' S_{ii'} \frac{(1-f_{i'}')}{(1-f_i)} \left[\frac{\mathcal{E}_{i'}' m_i}{\mathcal{E}_i m_{i'}'} \right]^{1/2} \delta(\mathcal{E}_{i'}' - \mathcal{E}_i) \, .
\end{aligned} \tag{A8}$$

Here the first and the second indices for q and q' designate the initial and final bands, respectively, involved in the transition.

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[*] Present address: Electronics and Telecommunications Research Institute, P.O. Box 106, Taejon, 305-600 Korea.

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