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Strong Correlation (T-Matrix) Effects in Electron–Hole Plasmas in Semiconductors

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The influence of strong coupling effects on the carrier–carrier scattering and dephasing rates in bulk semiconductors is investigated. We derive explicit expressions for the equilibrium and nonequilibrium scattering rates using a quantum kinetic approach in the T-matrix (full ladder) approximation. Numerical results are given, as example, for bulk GaAs in equilibrium using the T-matrix approach and, for a comparison, the Born approximation. Our results show the evidence for the influence of strong correlations. A reduction of the scattering rates by up to 30% compared to the Born result and the influence of resonances on the scattering cross sections are observed. The influence of strong correlations is shown to increase with decreasing temperature.

1. Introduction

The equilibrium and nonequilibrium properties of highly excited semiconductors are strongly influenced by the long-range Coulomb interaction between the free carriers, which leads to screening and strong correlations. Whereas the first effect has been studied in detail [1, 2], the relevance of the latter still remains unclear. From equilibrium quantum statistical theory, one anticipates that the conventional approach to the scattering and dephasing rates which is based on the Born approximation (scattering cross sections proportional to the square of the (dynamically) screened Coulomb potential) is strictly valid only in the limit of high or very low densities, $n > a_\mathrm{B}^{-3}$ or $n < (e^2/\varepsilon kT)^{-3}$, where a_B denotes the exciton Bohr radius and ε the background dielectric constant. For intermediate densities, strong correlations are expected to become important in the scattering quantities. These effects can be treated using a full T-matrix approach which includes the higher ladder terms beyond the Born approximation.

It is the goal of this paper to check the relevance of strong coupling (T-matrix) effects in bulk semiconductors quantitatively, based on a rigorous quantum mechanical treatment. Therefore, we derive expressions for the equilibrium and nonequilibrium scattering rates at the T-matrix level. The main input quantities of these expressions are the differential and total scattering cross sections which were calculated using a scattering phase shift analysis. This method is exact for nondegenerate systems, so we focus on the low density regime. In the last section of this paper, we compute the scattering rates and the carrier contribution to the dephasing rates for both, direct and exchange scattering processes, and compare them to the results of the Born approximation.

2. T-Matrix Scattering Rates

Using real time Green's function techniques, the following expression for the carrier scattering rates $\Sigma_a^{\gtrless}(\mathbf{p}\omega,\, t)$ in terms of the retarded T-matrix can be derived [3, 4]:

$$i\Sigma_a^{\gtrless}(\mathbf{p}_a\omega,\, t) = \pm \sum_b \frac{2(2\pi\hbar)^3}{V\hbar} \int \mathrm{d}\mathbf{p}_b\, \mathrm{d}\bar{\mathbf{p}}_a\, \mathrm{d}\bar{\mathbf{p}}_b\, 2\pi\, \delta(\omega + E_b(\mathbf{p}_b) - E_a(\bar{\mathbf{p}}_a) - E_b(\bar{\mathbf{p}}_b))$$
$$\times \frac{1}{2!}\, |\langle \mathbf{p}_a\mathbf{p}_b|\, \mathbf{T}_{ab}(\omega + E_b + i\epsilon)\, |\bar{\mathbf{p}}_b\bar{\mathbf{p}}_a\rangle^-|^2\, f_a^{\lessgtr}(\bar{\mathbf{p}}_a, t)\, f_b^{\gtrless}(\mathbf{p}_a, t)\, f_b^{\gtrless}(\mathbf{p}_b, t)\,. \tag{1}$$

Here, the abbreviations $f_a^< = f_a$ and $f_a^> = \pm(1 \pm f_a)$ are used. If the scattering rates are known, the damping of the one-particle states (dephasing rates) $\Gamma_a(\mathbf{p}\omega, t)$ can be calculated as

$$\begin{aligned}\Gamma_a(\mathbf{p}\omega, t) &= -2i\, \mathrm{Im}\, \Sigma_a^{\mathrm{R}}(\mathbf{p}\omega, t)\\ &= i[\Sigma_a^>(\mathbf{p}\omega, t) - \Sigma_a^<(\mathbf{p}\omega, t)]\,.\end{aligned} \tag{2}$$

In order to get the scattering rates needed, e.g., in the Markovian carrier–carrier scattering integrals of the Bloch equations, we confine the ω-dependence on the energy shell. Nonmarkovian generalisations of the T-matrix scattering integrals have been described by Kremp et al. [5].

The T-matrix as the main input quantity in formula (1) can be calculated by matrix inversion of the Lippmann-Schwinger equation [6] (operator notation)

$$\mathbf{T}_{ab}(\omega + i\epsilon) = \mathbf{V}_{ab} + \mathbf{V}_{ab}\, \frac{1 + f_a^< + f_b^<}{\omega - \mathbf{H}_{ab}^0 + i\epsilon}\, \mathbf{T}_{ab}(\omega + i\epsilon) \tag{3}$$

or by solving the effective Schrödinger equation using the methods of scattering theory. The latter approach is very efficient for nondegenerate systems (i.e. if the distributions $f^<$ in Eq. (3) can be neglected) and will be discussed in Section 3. As a result, the T-matrix is related to the differential scattering cross section by [7]

$$\frac{\mathrm{d}\sigma_{ab}(p,\, \Omega)}{\mathrm{d}\Omega} = (2\pi)^4\, \hbar^2 m_{ab}^2 \big|\langle \mathbf{p}|\, \mathbf{T}_{ab}\, |\bar{\mathbf{p}}\rangle^{\pm}\big|^2_{|\mathbf{p}| = |\bar{\mathbf{p}}|}\,. \tag{4}$$

Here, $\mathbf{p}$ is the momentum of relative motion, and $m_{ab} = m_a m_b/(m_a + m_b)$ denotes the reduced mass. We will use the second approach to evaluate the T-matrix in this paper.

To derive explicit expressions for the scattering rates from (1), we consider a nondegenerate electron–hole plasma in the spatially homogeneous case. Using relative and center of mass variables, we can write the T-matrix in the following form:

$$|\langle \mathbf{p}_a\mathbf{p}_b|\, \mathbf{T}_{ab}\, |\overline{\mathbf{p}_b}\,\overline{\mathbf{p}_a}\rangle^-|^2 = \frac{V}{(2\pi\hbar)^3}\, \delta(\mathbf{P} - \bar{\mathbf{P}})\, |\langle \mathbf{p}|\, \mathbf{T}_{ab}\, |\bar{\mathbf{p}}\rangle|^2\,. \tag{5}$$

Now we introduce the angles $\angle(\mathbf{p},\, \bar{\mathbf{p}}) = \vartheta$, $\angle(\mathbf{p},\, \mathbf{p}_1) = \vartheta_1$, and $\angle(\bar{\mathbf{p}},\, \mathbf{p}_1) = \vartheta_2$ with the abbreviations $\cos(\vartheta) = x$, $\cos(\vartheta_1) = x_1$, and $\cos(\vartheta_2) = x_2$. The angles are connected by the well-known relation of spherical trigonometry $x_2 = x x_1 + \sin(\vartheta)\, \sin(\vartheta_1)\, \cos(\varphi_x)$. With the assumption of isotropic distribution functions $f(p) = f(p^2)$, part of the integration can be performed, and we get for the scattering rates in the nondegenrate case

$$-i\Sigma_a^<(p_a,t) = \frac{4\pi}{(2\pi\hbar)^3}\,\frac{m_b^3}{m_{ab}^4}\int\limits_0^\infty \mathrm{d}p \int\limits_{-1}^{1} \mathrm{d}x_1 \int\limits_{-1}^{1} \mathrm{d}x \int\limits_0^{2\pi} \mathrm{d}\varphi_x\, p^3\,\frac{\mathrm{d}\sigma(p,\,\Omega)}{\mathrm{d}\Omega}$$
$$\times f_a(p_a^2 + 2p^2 - 2p_a p x_1 + 2p_a p x_2)$$
$$\times f_b(\gamma^2[p_a^2 + p^2 - p_a p x] + 2\gamma[p^2 x - p_a p x_2] + p^2)\,, \tag{6}$$

$$i\Sigma_a^>(p_a,t) = \frac{4\pi}{(2\pi\hbar)^3}\,\frac{m_b^3}{m_{ab}^4}\int\limits_0^\infty \mathrm{d}p \int\limits_{-1}^{1} \mathrm{d}x_1\, p^3\sigma^{\mathrm{tot}}(p)$$
$$\times f_b(\gamma^2 p_a^2 + (1+\gamma)^2\,p^2 - 2\gamma(1+\gamma)\,p_a p x_1)\,. \tag{7}$$

Here, $\gamma = m_b/m_a$ is the mass ratio, $\sigma^{\mathrm{tot}}(p)$ is the total cross section, and p denotes the modulus of the momentum of relative motion.

If the charged particles are in thermal equilibrium, we can use $f_b(p^2) = f_b^0(p^2) = (n_b\Lambda_b^3)/(2s_b+1)\,\exp\left[-p^2/2m_b k_{\mathrm{B}}T\right]$ in equation (7). $\Lambda_b = (2\pi\hbar^2/m_b k_{\mathrm{B}}T)^{1/2}$ is the thermal wavelength. In this case, a considerable simplification is possible, and it follows

$$i\Sigma_a^>(p_a) = \frac{4\pi}{(2\pi\hbar)^3}\,\frac{m_b^2 m_a}{m_{ab}^3}\,\frac{n_b\Lambda_b^3 k_{\mathrm{B}}T}{p_a}\int\limits_0^\infty \mathrm{d}p\, p^2\sigma^{\mathrm{tot}}(p)$$
$$\times \left[\mathrm{e}^{-(p_a/m_a - p/m_{ab})^2\, m_b/2k_{\mathrm{B}}T} - \mathrm{e}^{-(p_a/m_a + p/m_{ab})^2\, m_b/2k_{\mathrm{B}}T}\right]. \tag{8}$$

The scattering rate $\Sigma_a^<(p_a)$ can be calculated using the detailed balance, that means $\Sigma_a^<(p_a) = -\Sigma_a^>(p_a)\, f_a^0(p_a)$.

3. Scattering Cross Section

The scattering cross sections were determined using a phase shift analysis [8] (T-matrix approach) and, for comparison, using the well-known Born approximation. We have computed the scattering phase shifts δ_l by solving the radial Schrödinger equation with a statically screened Coulomb potential and self-energy shifts in Debye approximation [9]. This method is exact for nondegenerate systems which will be the situation of interest here. As a result, the differential cross section can be expressed in terms of the scattering phase shifts

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{\hbar^2}{p^2}\sum_{l,l'}^{\infty} (2l+1)\,(2l'+1)\,\sin(\delta_{l'})\,\sin(\delta_{l'})\,\cos(\delta_l - \delta_{l'})\,\mathbf{P}_l(\cos\vartheta)\,\mathbf{P}_{l'}(\cos\vartheta)\,, \tag{9}$$

where $\mathbf{P}_l(\cos\vartheta)$ are the Legendre polynomials, δ_l are the scattering phase shifts, and l denotes the quantum number of angular momentum. The total cross section for electron–hole scattering can be written as [7]

$$\sigma_{ab}^{\mathrm{tot}}(p) = \frac{4\pi\hbar^2}{p^2}\sum_{l=0}^{\infty} (2l+1)\,\sin^2(\delta_l) \qquad (a \neq b)\,. \tag{10}$$

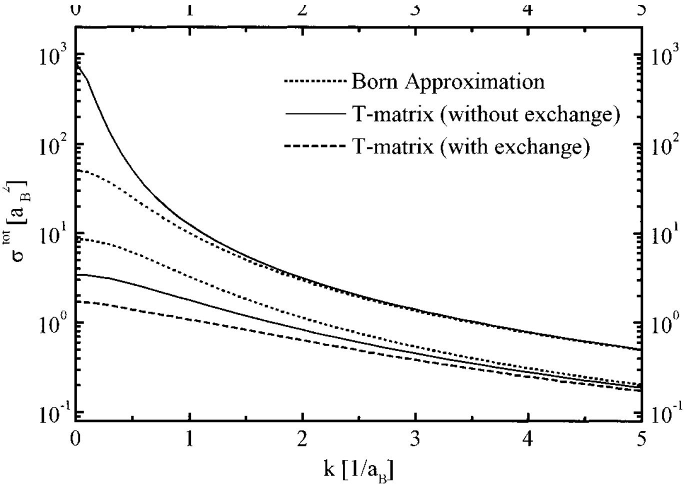

Fig. 1. Total scattering cross section for electron–hole scattering (upper pair of lines) and electron–electron scattering (lower triple of lines) in Born approximation and full T-matrix approach for an inverse Debye screening length $\varkappa = 1.0a_B^{-1}$

For electron–electron and hole–hole scattering, the exchange contribution has to be taken into account, i.e.

$$\sigma_{aa}^{\mathrm{tot}}(p) = \frac{2\pi\hbar^2}{p^2} \sum_{l=0,2,4\ldots}^{\infty} (2l+1)\,\sin^2(\delta_l) + \frac{6\pi\hbar^2}{p^2} \sum_{l=1,3,5\ldots}^{\infty} (2l+1)\,\sin^2(\delta_l)\,. \tag{11}$$

In Fig. 1, the total scattering cross sections for an electron–hole system with an inverse Debye length of $\varkappa = 1.0a_B^{-1}$ ($\varkappa^2 = 4\pi\Sigma_a n_a e^2/\varepsilon k_B T$) are shown. For low wave numbers, the full T-matrix calculation reduces the cross section compared to the Born result in the case of electron–electron scattering. The exchange contribution gives an additional reduction of the cross section, but for lower densities (smaller values of $\varkappa$) and for particles with larger mass (holes) the exchange can be neglected. As expected, the T-matrix and Born results coincide for high scattering energies. In the considered case of electron–hole scattering, the T-matrix result is larger than the Born result due to a s-wave resonance. However, for smaller values of $\varkappa$, there is no essential contribution due to resonances, and the T-matrix calculations give smaller cross section than the Born approximation.

4. Numerical Results and Discussion

To demonstrate the effect of strong correlations, we choose the electron–hole system in bulk GaAs with the following parameters: $m_e = 0.067m_0$ (m_0 vacuum electron mass), $a_B = 132$ Å, and a background dielectric constant $\varepsilon = 12.998$.

In Fig. 2, the total electron dephasing rate $\Gamma_{ee} + \Gamma_{eh}$ is plotted for three electron densities and a temperature of $T = 300$ K. For $n = 5.32 \times 10^{16}$ cm^{-3} (Fig. 2a), the T-matrix result is larger than the Born result due to the resonance effect (s-wave) in the electron–hole cross section (see Fig. 1) which enters the electron–hole rates $\Sigma_{eh}^{>}$ and $\Sigma_{eh}^{<}$. In

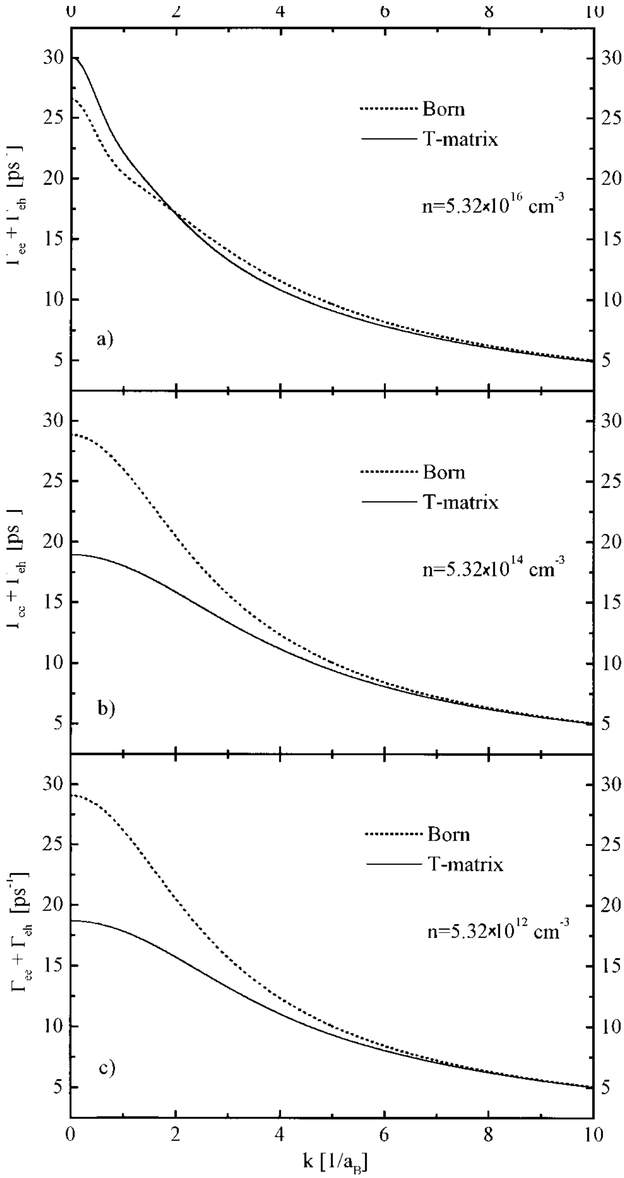

Fig. 2. Electron dephasing rate $\Gamma_{\rm ee} + \Gamma_{\rm eh}$ for different densities and $T = 300$ K in Born and T-matrix approximations

Figs. 2b, c, the full T-matrix gives a reduction compared to the Born result, especially for low external momenta p_a. For high momenta both approximation schemes coincide.

As expected, the deviations between T-matrix and Born approximation increase for lower temperatures. One can see this in Fig. 3, where the same quantity as in Fig. 2 is plotted for $T = 150$ K. The density is chosen in such a way that one has to use the same input cross section as in Fig. 2b (same $\varkappa$ value).

The density dependence of the scattering rates $\Sigma_a^>(p_a = 0)$ which determines $\Gamma_a(p_a = 0)$ in the low density region, is shown in Fig. 4. Again, one can observe the

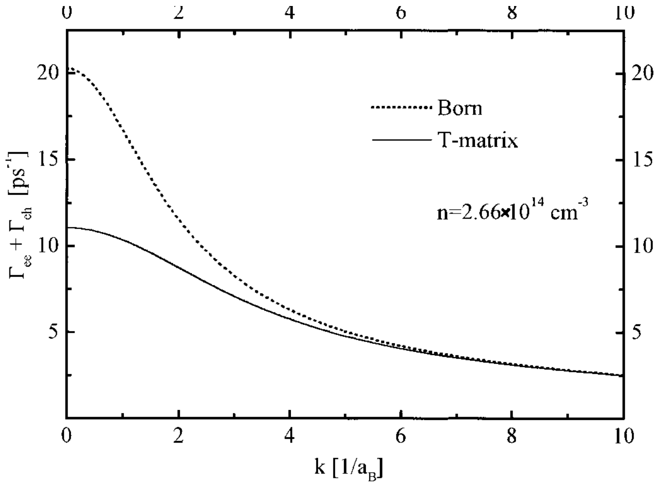

Fig. 3. Electron dephasing rate $\Gamma_{\text{ee}} + \Gamma_{\text{eh}}$ for $n = 2.66 \times 10^{14}$ cm^{-3} and $T = 150$ K (same input cross section as Fig. 2b)

reduction of the scattering rates due to higher ladder terms and the influence of resonance effects contained in the T-matrix approach. The increase of the T-matrix scattering rate $\Sigma^{>}_{\text{eh}}$ around $n = 1 \times 10^{17}$ cm^{-3} is due to the s-wave resonance in the cross section. As expected, the T-matrix results approach the Born approximation for higher densities, because the plasma becomes weakly coupled. At high densities (or low temperatures), the nondegenerate calculations are not quantitatively correct, but they are expected to reproduce the correct qualitative trend, in particular, the correct comparison to the Born approximation. To obtain accurate results in this regime, degeneracy effects (Pauli blocking factors) have to be taken into account in the scattering cross sections

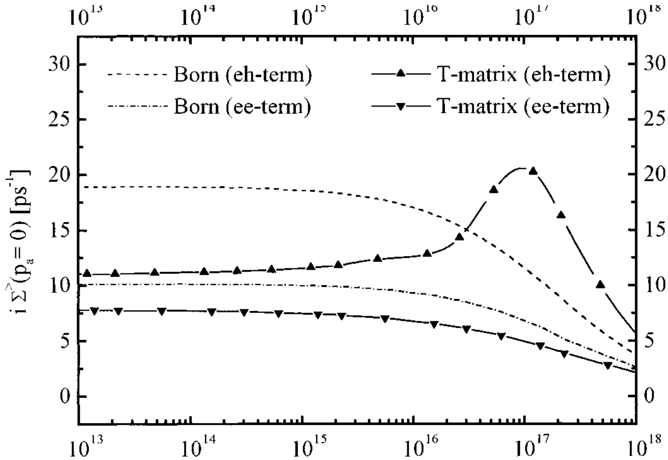

Fig. 4. Scattering rates $\Sigma^{>}_{\text{ee}}(p_a = 0)$ and $\Sigma^{>}_{\text{eh}}(p_a = 0)$ for $T = 300$ K as functions of the carrier density

(effective Schrödinger equation) and in the scattering rates. In this situation, the solution of the Lippmann-Schwinger equation (3) may be advantageous. However, as was shown in our analysis, strong T-matrix effects occur also at low densities, where the electron–hole plasma is nondegenerate. Here, the presented approach is simple and efficient, and allows, in particular, to calculate nonequilibrium scattering rates, too.

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