Field effect on the impact ionization rate in semiconductors

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Impact ionization plays a crucial role for electron transport in semiconductors at high electric fields. We derive appropriate quantum kinetic equations for electron transport in semiconductors within linear response theory. The field-dependent collision integral is evaluated for the process of impact ionization. A known, essentially analytical result is reproduced within the parabolic band approximation [W. Quade *et al.*, Phys. Rev. B **50**, 7398 (1994)]. Based on the numerical results for zero field strengths but realistic band structures, a fit formula is proposed for the respective field-dependent impact ionization rate. Explicit results are given for GaAs, Si, GaN, ZnS, and SrS. © *2000 American Institute of Physics.* [S0021-8979(00)03002-4]

I. INTRODUCTION

The study of high field transport in semiconductors has both theoretical interest and practical applications.[1] While electron scattering at other electrons, impurities, and phonons determines the low-field electron distribution function (EDF), intervalley electron-phonon scattering, and especially, band-to-band impact ionization become the dominant scattering processes for high fields in the mega volt per centimeter domain, leading to carrier multiplication and field clamping.[2]

We have previously calculated the impact ionization rate for Si and GaAs,[3] ZnS,[4–6] GaN,[7] and SrS (Ref. 8) neglecting the influence of the electric field on the collision term—the intracollisional field effect (ICFE). We have used a local empirical pseudopotential method (EPM) to calculate the band structure which has pronounced influence on the numerical results for the impact ionization rate. Therefore, nonlocal contributions to the pseudopotentials arising from different angular momentum states have been taken into account for ZnS.[5,6]

However, the ICFE should also affect the behavior of the impact ionization rate in the high-field regime. For instance, the evaluation of the Barker–Ferry kinetic equation[9] for Si[10] has indicated that the threshold energy for impact ionization is lowered due to the field because the impacting electron is further accelerated during the collision. This results in a higher ionization rate near the threshold, whereas for higher energies of the impacting electron the field influence vanishes.

Quade *et al.*[11] applied a density matrix approach to carrier generation in semiconductors. Within the parabolic band approximation, they were able to give an essentially analytical result for the field-assisted impact ionization rate which was evaluated for GaAs and Si. Again, the systematic lowering of the threshold energy with the field strength has been shown.

The field dependence of the collision integral was also studied by means of the Green function technique, solving the Kadanoff–Baym equations[12] in various approximations. Avoiding the conventional gradient expansion or delta-function approximation for the spectral density, an integral equation has been derived for the EDF taking into account the ICFE.[13,14] The Levinson[15] or Barker–Ferry transport equation[9] was evaluated within a saddle-point approximation for GaAs at high field strengths, taking into account electron-phonon interactions.[16] Alternatively, a gauge-invariant formulation of the Airy representation of the Kadanoff–Baym theory was developed.[17] The Mori projection operator technique was applied to study nonlinear transport in semiconductors and, especially, the ICFE and collision broadening.[18] The method of the nonequilibrium statistical operator as developed by Zubarev[19] was applied to study both steady-state and transient properties in hot-electron transport.[20,21]

We derive quantum kinetic equations for the EDF in semiconductors using the Zubarev approach and take into account the full field dependence of the collision integral. We then focus on impact ionization processes and rederive the general, field-dependent impact ionization rate given by Quade *et al.*[11] within the parabolic band approximation, and the Keldysh formula[22] valid for energies near the threshold. Comparing with the results for the zero-field impact ionization rate which were calculated with realistic band

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structures,[4–8] a field-dependent fit formula is proposed. Explicit results are given for various semiconductor materials.

II. DERIVATION OF A QUANTUM KINETIC EQUATION

Quantum kinetic equations can be derived within different methods of nonequilibrium statistical physics. For instance, the Green function technique has been successfully applied to derive the well-known Kadanoff–Baym equations.[12] Alternatively, the response method allows to derive balance equations for the single-particle density matrix where the time evolution of correlations is described by the nonequilibrium statistical operator (NESO). This method, developed mainly by Zubarev,[19] has been applied to charged particle systems such as plasmas and semiconductors.[23] Starting point is a modified Liouville–von Neumann equation for the NESO $\varrho(t)$ which is governed by the Hamilton operator $H(t)$

$$\frac{\partial}{\partial t}\varrho(t)+\frac{1}{i\hbar}[\varrho(t),H(t)]=-\lim_{\varepsilon\to+0}\varepsilon[\varrho(t)-\varrho_{\mathrm{rel}}(t)].$$ (1)

This equation has a formal solution of the form

$$\varrho(t)=\varrho_{\mathrm{rel}}(t)-\int_{-\infty}^{t}dt'\,e^{\varepsilon(t'-t)}U(t,t')\left\{\frac{\partial}{\partial t'}\varrho_{\mathrm{rel}}(t')\right.$$
$$\left.+\frac{1}{i\hbar}[\varrho_{\mathrm{rel}}(t'),H(t')]\right\}U^{\dagger}(t,t').$$ (2)

The time dependence of operators is given in the Heisenberg picture via the time evolution operator $U(t,t')$

$$A(t,t')=U^{\dagger}(t,t')AU(t,t'),$$
$$U(t,t')=\mathcal{T}\exp\left[-\frac{i}{\hbar}\int_{t'}^{t}H(\tau)d\tau\right],$$ (3)

where $\mathcal{T}$ is the time-ordering operator. The relevant statistical operator $\varrho_{\mathrm{rel}}(t)$ is usually taken as a generalized Gibbs state as proposed by Robertson[24]

$$\varrho_{\mathrm{rel}}(t)=\exp\left[-\Phi(t)-\sum_{m}F_{m}(t)B_{m}\right],$$ (4)

where $\Phi(t)$ is the normalization, and the Lagrange parameters $F_{m}(t)$ are determined by the self-consistency conditions

$$\langle B_{m}\rangle^{t}=\mathrm{Tr}[\varrho(t)B_{m}]\equiv\langle B_{m}\rangle_{\mathrm{rel}}^{t}=\mathrm{Tr}[\varrho_{\mathrm{rel}}(t)B_{m}].$$ (5)

Quantum kinetic equations are immediately derived for any relevant observable B_{m} which is not explicitly time dependent by performing the time derivative according to

$$\frac{d}{dt}\langle B_{m}\rangle^{t}=\mathrm{Tr}\left\{\frac{1}{i\hbar}[B_{m},H(t)]\varrho(t)\right\}\equiv\langle\dot{B}_{m}\rangle^{t}.$$ (6)

The first method is to insert the NESO Eq. (2) which is mainly determined by the relevant statistical operator (4). This leads to a Boltzmann-type balance equation for the relevant observables with a drift and a collision term. The second method is to apply perturbation theory in situations where the Hamilton operator can be split according to $H(t)$

$=H^{0}(t)+H'$. The main part $H^{0}(t)$ contains the ideal contributions and the full time variation of, e.g., external fields, whereas the perturbation H' describes the interactions. The following quantum kinetic equation is then derived:

$$\frac{\partial}{\partial t}\langle B_{m}\rangle^{t}-i\sum_{n}\Omega_{mn}(t)\langle B_{n}\rangle^{t}=J_{m}(t),$$

$$\frac{1}{i\hbar}[B_{m},H^{0}(t)]=i\sum_{n}\Omega_{mn}(t)B_{n},$$ (7)

$$\frac{1}{i\hbar}\langle[B_{m},H']\rangle^{t}=\mathrm{Tr}\left\{\varrho(t)\frac{1}{i\hbar}[B_{m},H']\right\}\equiv J_{m}(t).$$

Since the explicit time dependence of operators is now only determined by $H^{0}(t)$, a corresponding time evolution operator can be introduced via

$$U_{0}(t,t')=\mathcal{T}\exp\left[-\frac{i}{\hbar}\int_{t'}^{t}H^{0}(\tau)d\tau\right],$$ (8)

so that the NESO Eq. (2) can be given after partial integration of the Liouville–von Neumann Eq. (1) in the form

$$\varrho(t)=\varrho_{\mathrm{rel}}(t)-\int_{-\infty}^{t}dt'\,e^{\varepsilon(t'-t)}U_{0}(t,t')$$
$$\times\left\{\frac{\partial}{\partial t'}\varrho_{\mathrm{rel}}(t')+\frac{1}{i\hbar}[\varrho_{\mathrm{rel}}(t'),H^{0}(t')]\right.$$
$$\left.+\frac{1}{i\hbar}[\varrho(t'),H']\right\}U_{0}^{\dagger}(t,t').$$ (9)

The interaction part H' contributes via the full NESO $\varrho(t')$ so that only an iterative solution of the quantum kinetic Eq. (7) is possible. Furthermore, Eq. (9) contains the full time evolution of the relevant statistical operator $\varrho_{\mathrm{rel}}(t')$ which is determined by the mean values of the relevant observables B_{n}. The time evolution of the system at all former time steps is contained in the integration in Eq. (9) which is usually denoted as memory effect. The corresponding time derivative $(\partial/\partial t')\varrho_{\mathrm{rel}}(t')$ is given by the time variation of the mean values according to

$$\frac{\partial}{\partial t}\varrho_{\mathrm{rel}}(t)+\frac{1}{i\hbar}[\varrho_{\mathrm{rel}}(t),H^{0}(t)]=\sum_{n}\frac{\delta\varrho_{\mathrm{rel}}(t)}{\delta\langle B_{n}\rangle^{t}}J_{n}(t). \quad (10)$$

The commutator $[\varrho_{\mathrm{rel}}(t'),H^{0}(t')]$ cancels in Eq. (9) and we have finally the following equation for the NESO:

$$\varrho(t)=\varrho_{\mathrm{rel}}(t)-\int_{-\infty}^{t}dt'\,e^{\varepsilon(t'-t)}U_{0}(t,t')$$
$$\times\left\{\sum_{n}\frac{\delta\varrho_{\mathrm{rel}}(t')}{\delta\langle B_{n}\rangle^{t'}}J_{n}(t')\right.$$
$$\left.+\frac{1}{i\hbar}[\varrho(t'),H']\right\}U_{0}^{\dagger}(t,t').$$ (11)

Inserting this expression into Eq. (7) and iterating up to the second order with respect to H', the following general quantum kinetic equation is derived:[25]

$$\frac{\partial}{\partial t}\langle B_m\rangle^t - i\sum_n \Omega_{mn}(t)\langle B_n\rangle^t = J_m^{(1)}(t) + J_m^{(2)}(t),$$

$$J_m^{(1)}(t) = \frac{1}{i\hbar}\langle [B_m, H']\rangle_{\text{rel}}^t, \tag{12}$$

$$J_m^{(2)}(t) = -\frac{1}{\hbar^2}\int_{-\infty}^t dt'\, e^{\varepsilon(t'-t)}$$

$$\times\left\{\left[H',[H'(t,t'),B_m(t,t')]\right.\right.$$

$$\left.\left. + i\hbar\sum_n B_n\frac{\delta J_m^{(1)}(t,t')}{\delta\langle B_n\rangle_{\text{rel}}^{t'}}\right]\right|_{t'}^{t'}\bigg\}_{\text{rel}}.$$

This equation contains the interactions up to the second order, memory effects via $\varrho_{\text{rel}}(t')$ which is determined by the mean values $\langle B_n\rangle^{t'}$, and the effects of an external, time-dependent field via $H^0(t)$ (for a more detailed discussion, see Ref. 23). If the Hamilton operator H^0 is not explicitly time dependent, the second-order collision operator $J_m^{(2)}(t)$ in the quantum kinetic Eq. (12) can be given in a Markovian form[26,27]

$$J_m^{(2,M)}(t) = -\frac{1}{\hbar^2}\int_{-\infty}^0 dt_1 e^{\varepsilon t_1}\left\langle\left[H'(t_1),[H',B_m]\right.\right.$$

$$\left.\left. + i\hbar\sum_k B_k\frac{\delta J_m^{(1)}(t)}{\delta\langle B_k\rangle^t}\right]\right\rangle_{\text{rel}}^t. \tag{13}$$

III. SEMICONDUCTOR IN A HOMOGENEOUS ELECTRIC FIELD

After we have outlined the derivation of a general quantum kinetic Eq. (12) by means of the NESO Eq. (11), we will now apply the formalism to treat the electron transport in semiconductors at high electric field strengths. We start with the Hamilton operator for electrons in an electromagnetic field. The vector potential $\vec{A}(\vec{r},t)$ determines the electric and magnetic fields according to

$$\vec{E}(\vec{r},t) = -\nabla\varphi(\vec{r},t) - \frac{1}{c}\frac{\partial\vec{A}(\vec{r},t)}{\partial t},$$

$$\vec{B}(\vec{r},t) = \nabla\times\vec{A}(\vec{r},t). \tag{14}$$

Supposing a homogeneous electromagnetic field, i.e., $\vec{A}(t) = \vec{A}_0\cos(\omega t + \alpha_0)$, the electrons couple only to the electric field component and $\vec{B} = 0$. Choosing the gauge transformation $\varphi(\vec{r},t) = 0$, the electric field is given by $\vec{E}(\mathbf{t}) = \vec{E}_0\sin(\omega t + \alpha_0)$ with $\vec{E}_0 = \vec{A}_0\omega/c$. The Hamilton operator

$$H(t) = H_{\text{el}}^0(t) + H_{\text{ph}}^0 + H_{e-i}' + H_{e-ph}' + H_{e-e}' \tag{15}$$

consists of the electrons in the band ν coupled to the field, the phonons, the electron-impurity interaction via a potential Φ, the electron–phonon interaction in Fröhlich representation with a matrix element D_q, and the electron–electron interaction V_{ee}

$$H_{\text{el}}^0(t) = \sum_{\nu p}\left[\varepsilon_{\nu p} - \frac{e}{m_\nu c}\vec{p}\cdot\vec{A}_0\cos(\omega t + \alpha_0)\right.$$

$$\left. + \frac{e^2}{2m_\nu c^2}A_0^2\cos^2(\omega t + \alpha_0)\right]a_{\nu p}^\dagger a_{\nu p},$$

$$H_{\text{ph}}^0 = \sum_q \hbar\omega_q b_q^\dagger b_q,$$

$$H_{e-i}' = \frac{1}{V}\sum_{\nu p,\nu' p'}\Phi(p,p')a_{\nu p}^\dagger a_{\nu' p'}, \tag{16}$$

$$H_{e-ph}' = \frac{1}{\sqrt{V}}\sum_{\nu pq} D_q(b_q + b_{-q}^\dagger)a_{\nu,p+\hbar q}^\dagger a_{\nu p},$$

$$H_{e-e}' = \frac{1}{2}\sum_{\nu_1\nu_2,\nu_1'\nu_2'}\sum_{k_1 k_2, k_1' k_2'}$$

$$\times V_{ee}(k_1'k_2',k_1 k_2)a_{\nu_2'k_2'}^\dagger a_{\nu_1'k_1'}^\dagger a_{\nu_1 k_1} a_{\nu_2 k_2}.$$

$a_{\nu p}^\dagger$, $a_{\nu p}$ and $b_q^\dagger$, b_q are creation and annihilation operators for electrons in the band ν and phonons, respectively. Effective masses m_ν can be introduced for spherical parabolic bands, i.e., $\varepsilon_{\nu p} = \hbar^2 p^2/2m_\nu$.

We have to specify the relevant observables B_m for the treatment of electron transport in semiconductors. For a complete description of the coupled electron-phonon system, we have to take into account the single-particle occupation numbers $n_\nu(p)$ for the valence ($\nu = v$) and the conduction bands ($\nu = c$) as well as the phonon occupation numbers $N(q)$ as relevant observables, i.e., $\{B_m\} = \{n_\nu(p), n_c(p), N(q)\}$. Their mean values are the electron single-particle distribution function and the phonon distribution function, respectively,

$$f_{\nu p}(t) = \langle n_\nu(p)\rangle_{\text{rel}}^t = \langle a_{\nu p}^\dagger a_{\nu p}\rangle_{\text{rel}}^t,$$

$$N_q(t) = \langle N(q)\rangle_{\text{rel}}^t = \langle b_q^\dagger b_q\rangle_{\text{rel}}^t. \tag{17}$$

In what follows, we will restrict ourselves to the treatment of the EDF. However, also the evolution of the phonon distribution function can be studied. The EDF can be related to the diagonal part of the Wigner distribution function and is determined from the general quantum kinetic Eq. (12)

$$\frac{\partial}{\partial t}f_{\nu p}(t) + e\vec{E}(t)\cdot\frac{\partial}{\partial\vec{p}}f_{\nu p}(t) = J_e(p,t). \tag{18}$$

We have to evaluate the field-dependent collision terms $J_e(p,t)$ given by Eq. (12). It follows immediately from the Hamilton operator (16) that

$$J_e^{(1)}(p,t) = \frac{1}{i\hbar}\{[n_\nu(p),H']\}_{\text{rel}}^t = 0. \tag{19}$$

Therefore, the second-order collision terms $J^{(2)}(t)$ in Eq. (12) can be evaluated from the Markovian form Eq. (13) in which the time-dependent operators are given in the Heisenberg representation Eq. (3) using the time evolution operator (8). The following second-order electron collision terms for the scattering at impurities, with phonons and with other electrons is then derived (for details, see Ref. 23)

$$J_e^{(2,e-i)}(p,t) = -\frac{2}{\hbar^2 V^2} \sum_{\nu'p'} |\Phi(p',p)|^2$$

$$\times \int_{-\infty}^t dt' e^{\varepsilon(t'-t)} \cos[\Omega_{\nu p,\nu'p'}(t,t')]$$

$$\times [f_{\nu'p'}(t) - f_{\nu p}(t)], \tag{20}$$

$$J_e^{(2,e-ph)}(p,t) = -\frac{2}{\hbar^2 V} \sum_q |D_q|^2 \int_{-\infty}^t dt' e^{\varepsilon(t'-t)}$$

$$\times \{[(1+N_q)f_{\nu p+q}(t)[1-f_{\nu p}(t)]$$

$$-N_q f_{\nu p}(t)[1-f_{\nu p+q}(t)]]$$

$$\times \cos[\Omega_{\nu p,\nu p+\hbar q}(t,t') + \omega_q(t-t')]$$

$$+[N_q f_{\nu p-q}(t)[1-f_{\nu p}(t)] - (1+N_q)$$

$$\times f_{\nu p}(t)[1-f_{\nu p-q}(t)]]$$

$$\times \cos[\Omega_{\nu p,\nu p-\hbar q}(t,t') - \omega_q(t-t')]\}, \tag{21}$$

$$J_e^{(2,e-e)}(p,t) = -\frac{4}{\hbar^2} \sum_{\nu_2 \nu_1' \nu_2'} \sum_{k_2 k_1' k_2'} |V_{ee}(k_1'k_2',pk_2)|^2$$

$$\times \int_{-\infty}^t dt' e^{\varepsilon(t'-t)} \cos[\Omega_{\nu_1'k_1'\nu_2'k_2',\nu p\nu_2 k_2}(t,t')]$$

$$\times \{f_{\nu p}(t)f_{\nu_2 k_2}(t)[1-f_{\nu_1'k_1'}(t)][1-f_{\nu_2'k_2'}(t)]$$

$$-f_{\nu_1'k_1'}(t)f_{\nu_2'k_2'}(t)[1-f_{\nu p}(t)][1-f_{\nu_2 k_2}(t)]\}. \tag{22}$$

The quantities Ω are given by

$$\Omega_{\nu_1 k_1,\nu_2 k_2}(t,t') = \frac{1}{\hbar}(\varepsilon_{\nu_1 k_1} - \varepsilon_{\nu_2 k_2})(t-t') + \frac{\lambda_{\nu_1 k_1} - \lambda_{\nu_2 k_2}}{\hbar\omega}$$

$$\times [\sin(\omega t + \alpha_0) - \sin(\omega t + \alpha_0)] + \frac{e^2 A_0^2}{2\hbar c^2}$$

$$\times \left(\frac{1}{m_{\nu_1}} - \frac{1}{m_{\nu_2}}\right)\left[\frac{t-t'}{2} + \frac{\sin(2\omega t + 2\alpha_0)}{4\omega}\right.$$

$$\left. - \frac{\sin(2\omega t' + 2\alpha_0)}{4\omega}\right], \tag{23}$$

$$\Omega_{\nu_1'k_1'\nu_2'k_2',\nu_1 k_1 \nu_2 k_2}(t,t') = \frac{1}{\hbar}(\varepsilon_{\nu_1'k_1'} + \varepsilon_{\nu_2'k_2'} - \varepsilon_{\nu_1 k_1} - \varepsilon_{\nu_2 k_2})$$

$$\times (t-t')$$

$$+ \frac{\lambda_{\nu_1'k_1'} + \lambda_{\nu_2'k_2'} - \lambda_{\nu_1 k_1} - \lambda_{\nu_2 k_2}}{\hbar\omega}$$

$$\times [\sin(\omega t + \alpha_0) - \sin(\omega t' + \alpha_0)]$$

$$+ \frac{e^2 A_0^2}{2\hbar c^2}\left(\frac{1}{m_{\nu_2'}} + \frac{1}{m_{\nu_1'}} - \frac{1}{m_{\nu_1}}\right.$$

$$\left. - \frac{1}{m_{\nu_2}}\right)\left[\frac{t-t'}{2} + \frac{\sin(2\omega t + 2\alpha_0)}{4\omega}\right.$$

$$\left. - \frac{\sin(2\omega t' + 2\alpha_0)}{4\omega}\right]. \tag{24}$$

The coupling of the electrons to the external field is described by $\lambda_{\nu p} = -e\vec{p}\cdot\vec{A}_0/cm_\nu$. The last terms on the right-hand side of Eqs. (23) and (24) vanish for intraband processes, but give contributions for interband processes (impact ionization) considered in the next section.

For constant electric fields, i.e., $\vec{E}_0 = const.$ and $\omega \to 0$, the quantities $\vec{A}_0 = \vec{E}_0 c/\omega$ and $\lambda_{\nu p}$ diverge. The respective singularities in the collision integrals can be removed by replacing the Wigner functions $f^W(\vec{p},t)$ by gauge-invariant functions $f^G(\vec{p},t)$ according to[23]

$$f_{\nu p}(t) = f_\nu^G(\vec{p},t) \equiv f_\nu^W[\vec{P}(t)], \tag{25}$$

where $\vec{P}(t) = \vec{p} + e\vec{A}(t)/c$ is the canonical momentum. The quantities Eqs. (23) and (24) reduce then to their static values,

$$\Omega_{\nu_1 k_1,\nu_2 k_2}^0(t,t') = \frac{1}{\hbar}(\varepsilon_{\nu_1 k_1} - \varepsilon_{\nu_2 k_2})(t-t') - \frac{e\vec{E}}{2\hbar}$$

$$\cdot \left(\frac{\vec{k}_1}{m_{\nu_1}} - \frac{\vec{k}_2}{m_{\nu_2}}\right)(t-t')^2$$

$$+ \frac{1}{3}\omega_{F,i}^3(t-t')^3, \tag{26}$$

$$\Omega_{\nu_1'k_1'\nu_2'k_2',\nu_1 k_1 \nu_2 k_2}^0(t,t') = \frac{1}{\hbar}(\varepsilon_{\nu_1'k_1'} + \varepsilon_{\nu_2'k_2'} - \varepsilon_{\nu_1 k_1}$$

$$- \varepsilon_{\nu_2 k_2})(t-t') - \frac{e\vec{E}}{2\hbar}\cdot\left(\frac{\vec{k}'_1}{m_{\nu_1'}}\right.$$

$$+ \frac{\vec{k}'_2}{m_{\nu_2'}} - \frac{\vec{k}_1}{m_{\nu_1}} - \frac{\vec{k}_2}{m_{\nu_2}}\right)(t-t')^2$$

$$+ \frac{1}{3}\omega_{F,e}^3(t-t')^3, \tag{27}$$

where $\vec{E} = \vec{E}_0 \sin(\alpha_0)$ and

$$\omega_{F,i}^3 = \frac{e^2 E^2}{2\hbar}\left(\frac{1}{m_{\nu_1}} - \frac{1}{m_{\nu_2}}\right),$$

$$\omega_{F,e}^3 = \frac{e^2 E^2}{2\hbar}\left(\frac{1}{m_{\nu_1'}} + \frac{1}{m_{\nu_2'}} - \frac{1}{m_{\nu_1}} - \frac{1}{m_{\nu_2}}\right). \tag{28}$$

IV. IMPACT IONIZATION RATE

The electron–electron collision integral Eq. (22) is studied in more detail. We are especially interested in the inelastic process of impact ionization which has a strong influence on the EDF at high electric field strengths. Previous calculations for Si and GaAs,[3,28] ZnS,[4–6] GaN,[7,29,30] SrS,[7,8] and InN[31] have indicated that substantial contributions to the im-
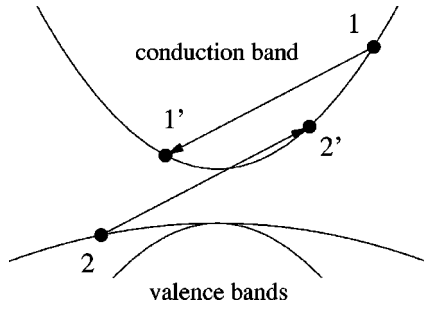
FIG. 1. Schematic impact ionization process for electrons.

pact ionization rate $r_{ii}(p)$ arise from electrons in the higher bands, especially for the wide band gap materials, so that we have taken into account four (to six) conduction bands and four valence bands, i.e., $\nu_i, \nu_i' = 1-4(6)$.

In the process of impact ionization, a conduction band electron impact ionizes a valence band electron, i.e., $1+2 \rightarrow 1'+2'$, see Fig. 1. The band indices and energies $\nu_1, \varepsilon_{k_1}, \nu_{1'}, \varepsilon_{k_1'}, \nu_{2'}, \varepsilon_{k_2'}$ run over the conduction bands, while ν_2, ε_{k_2} belong to the valence bands. Supposing that the semiconductor is not highly excited, the conduction bands are almost empty so that the Pauli blocking factors are unity, i.e., $(1-f_{\nu p}) \approx 1$. Furthermore, the (second) in-scattering term can be neglected compared with the (first) out-scattering term in the balance for the population of states with momentum p and the following collision integral can be given for field-dependent impact ionization:

$$J_e^{(2,ii)}(p,E_0,t) = -r_{ii}(p,E_0,t)f^W(p-eE_0t),$$

$$r_{ii}(p,E_0,t) = -\frac{4}{\hbar^2} \sum_{\nu_2\nu_1'\nu_2'} \sum_{k_2k_1'k_2'} |V_{ee}(k_1'k_2',pk_2)|^2$$

$$\times \int_{-\infty}^{t} dt' \, e^{\varepsilon(t'-t)} \cos[\Omega^0_{\nu_1'k_1'\nu_2'k_2',\nu p \nu_2 k_2}(t,t')]. \quad (29)$$

The matrix element contains the Debye-like screened Coulomb potential with the inverse screening length λ and the overlap (or Bloch) integrals $F_{ij}(k,q)$ for the impact ionization process

$$|V_{ee}(q)|^2 = \left(\frac{e^2}{\varepsilon\varepsilon_0 V_g}\right)^2 \left(\frac{F_{cc}F_{cv}}{q^2+\lambda^2}\right)^2 \delta_{k_1'+k_2'-p-k_2}, \quad (30)$$

ε and ε_0 are the relative and absolute permittivity, and V_g is the crystal volume.

We evaluate Eq. (29) for a direct semiconductor with spherical parabolic bands and effective masses for the valence $(m_{\nu_2} = m_\nu)$ and conduction band $(m_{\nu_1'} = m_{\nu_2'} = m_{\nu_1} = m_c)$, and define $\alpha = m_c/m_\nu$ and $\mu = (1+2\alpha)/(1+\alpha)$. Quade *et al.*[11] derived a collision integral similar to Eq. (29) within a density matrix approach and were able to evaluate the integrations over the momenta k_1' and k_2' essentially analytically in the Markov limit, considering the full, statically screened Coulomb matrix element between the two electrons. Following their derivation, we obtain with the definition of the Airy function

$$\frac{\pi}{(3a)^{1/3}} \text{Ai}\left(\pm\frac{x}{(3a)^{1/3}}\right) = \int_0^\infty d\tau \cos(a\tau^3 \pm x\tau) \quad (31)$$

the general result

$$r_{ii}^{(Q)}(p,E_0) = \frac{1}{\tau_Q} \int_0^\infty dE \bar{S}(E_p, E_p$$

$$-E)\frac{1}{E_F^{ii}} \text{Ai}\left(\frac{E_{\text{th}}-E_p+E}{E_F^{ii}}\right),$$

$$\frac{1}{\tau_Q} = \frac{\sqrt{\mu}}{4\pi^2(1+\alpha)^{3/2}} \left(\frac{e^2 F_{cv}F_{cc}\sqrt{m_c}}{\varepsilon\varepsilon_0\hbar^{3/2}}\right)^2,$$

$$\bar{S}(E_p,E) = \frac{1}{2}\left(\sqrt{\frac{E_M(E_p,E_\lambda,E)}{E_p}} + \sqrt{\frac{E_p}{E_M(E_p,E_\lambda,E)}}\right)$$

$$-1,$$

$$E_M(E_p,E_\lambda,E) = \frac{1}{2}(\sqrt{(E_\lambda-E)^2+4E_pE_\lambda}-E_\lambda+E),$$

$$E_p = \frac{p^2}{2m_c}, \quad E_\lambda = \mu^2\frac{\hbar^2\lambda^2}{2m_c}, \quad E_{\text{th}} = \mu E_g,$$

$$E_F^{ii} = \hbar\omega_F^{ii}, \quad \omega_F^{ii} = \left(\frac{(1+\alpha)(eE_0)^2}{8m_c\hbar}\right)^{1/3}. \quad (32)$$

E_p is the kinetic energy of the impacting electron, E_{th} is the threshold energy for impact ionization, E_g is the gap energy and ω_F^{ii} the electro-optical frequency. As a result of the field influence during the collision, the threshold energy for impact ionization is lowered, and the impact ionization rate increases significantly in this energy domain as shown by Quade *et al.*[11] for Si and GaAs explicitly. In the zero-field limit, the Airy function yields a delta function and we have simply

$$r_{ii}^{(Q)}(p,0) = \frac{1}{\tau_Q} \bar{S}(E_p,E_{\text{th}}). \quad (33)$$

Another analytical result for the impact ionization rate was derived by Keldysh[22] assuming a constant, i.e., q-independent matrix element $|V|$, and expanding the energies of the electrons involved in the process with respect to the threshold energy E_{th}. If we perform only the constant matrix element approximation but take into account the full field dependence of the collision integral Eq. (29), a modified impact ionization rate can be derived

$$r_{ii}^{(K)}(p,E_0) = \frac{1}{\tau_K} \int_0^\infty dE \left(\frac{E}{E_{\text{th}}}\right)^2 \frac{1}{E_F^{ii}} \text{Ai}\left(\frac{E_{\text{th}}-E_p+E}{E_F^{ii}}\right),$$

$$\frac{1}{\tau_K} = \frac{1}{32\pi^2(1+2\alpha)^{3/2}} \left(\frac{e^2 F_{cc}F_{cv}\sqrt{m_c}}{\varepsilon\varepsilon_0\hbar^{3/2}}\right)^2. \quad (34)$$

Again, the zero-field limit can be performed and we obtain the original Keldysh formula for impact ionization[22] which has frequently been used in simulation studies of electron transport in semiconductors (see, e.g., Ref. 32)

$$r_{ii}^{(K)}(p,0) = \frac{1}{\tau_K}\left(\frac{E_p-E_{\text{th}}}{E_{\text{th}}}\right)^2. \quad (35)$$

TABLE I. Parameters for the field dependent impact ionization rate Eq. (37) for various semiconductor materials, see Ref. 33. The band structure was determined within the EPM; nonlocal corrections were considered for ZnS and SrS.

	E_{th} (eV)	C ($10^{10}\,\mathrm{eV}^{-a}\,\mathrm{s}^{-1}$)	a
Si	0.8	36.22	3.683
GaAs	1.8	93.659	4.743
GaN	3.6	0.009 49	7.434
ZnS	3.8	5.935	5.073
SrS	4.0	59.723	3.182

The impact-ionization mean free flight time τ_K depends only on the effective masses, the relative permittivity and the overlap integrals, which are set equal to unity in Eq. (35). In principle, this prefactor $1/\tau_K$ cannot be taken as a free, adjustable parameter in simulations of high-field transport.

However, we have shown in previous articles[4–8] that the full band structure has to be considered when calculating the impact ionization rate in the zero-field limit where the time integration in Eq. (29) yields the energy-conserving delta function. The model of two parabolic bands applied so far is not sufficient to describe interband transitions, especially in wide band gap materials like ZnS, GaN, or SrS, where pronounced contributions arise from higher conduction bands. Four to six conduction bands (and four valence bands) are usually considered for the complete numerical evaluation of the zero-field impact ionization rate. These numerical results can be parameterized again in terms of a generalized Keldysh formula according to

$$r_{ii}^{(F)}(p,0) = C\left(\frac{E_p - E_{th}}{E_{th}}\right)^a, \quad (36)$$

where the prefactor C, the threshold energy E_{th}, and the power a are given in Table I for a variety of semiconductor materials. Obviously, the influence of the band structure manifests itself in values $a > 2$ compared with the original Keldysh formula (35) derived for spherical parabolic bands. Comparing Eqs. (34)–(36), we propose a new fit formula for impact ionization that considers the influence of an applied electric field and the full band structure according to

$$r_{ii}^{(F)}(p,E_0) = C\int_0^\infty dE\left(\frac{E}{E_{th}}\right)^a \frac{1}{E_F^{ii}}\mathrm{Ai}\left(\frac{E_{th} - E_p + E}{E_F^{ii}}\right). \quad (37)$$

In Fig. 2, we compare the numerical results according to Eq. (37) for GaAs with the parabolic band approximation of Quade *et al.*,[11] Eq. (32). The consideration of the full band structure (F) which is represented by the parameter a in Eq. (37) leads to a higher threshold compared with the parabolic band approximation (P) because the lowest conduction band in GaAs does not contribute to the impact ionization rate.[3] Furthermore, the full-band rate reaches higher values for medium energies due to the consideration of higher conduction bands. The applied electric field leads to a lowering of the threshold energy, but has no influence for energies above 2.5 eV.

The results for Si are shown in Fig. 3. Bude *et al.*[10] solved the Barker–Ferry equation and gave results for the
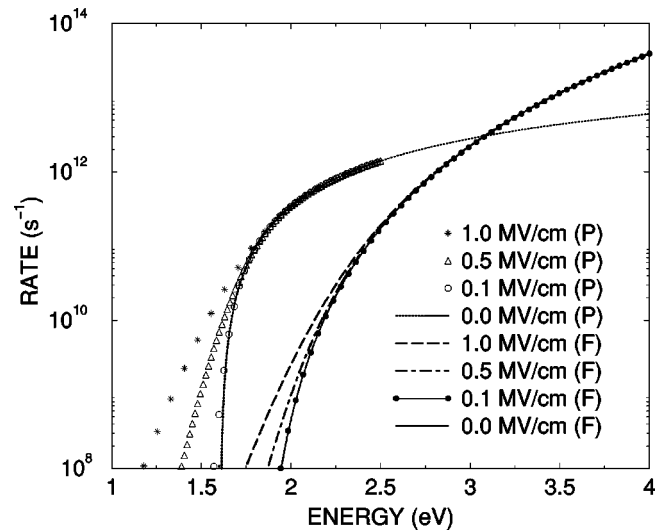

FIG. 2. Field dependent impact ionization rate for GaAs within the parabolic band approximation (see Ref. 11) (P) according to Eq. (32) compared with Eq. (37) where the full band structure (F) is considered.

field-dependent impact ionization rate in Si including the effect of high scattering rates, i.e., collision broadening, for energies above 1.5 eV. Both effects lead to a lowering of the threshold energy and to an increase of the impact ionization rate so that it is not surprising that their results lie above our curves. However, the energy conserving δ function was replaced by a Lorentzian whose extended tails might overestimate the effect. Furthermore, no results were given for the actual threshold region.

Quade *et al.*[11] showed field dependent rates also for Si along the (001) direction (see Fig. 7 of their article). The threshold energy is lowered from 1.1 to 0.9 eV for the same field strength domain of 0.1 to 1.0 MV/cm, and the curves show a stronger increase compared with the present results, i.e., a *harder* threshold behavior. This underlines the necessity to include more details of the band structure.
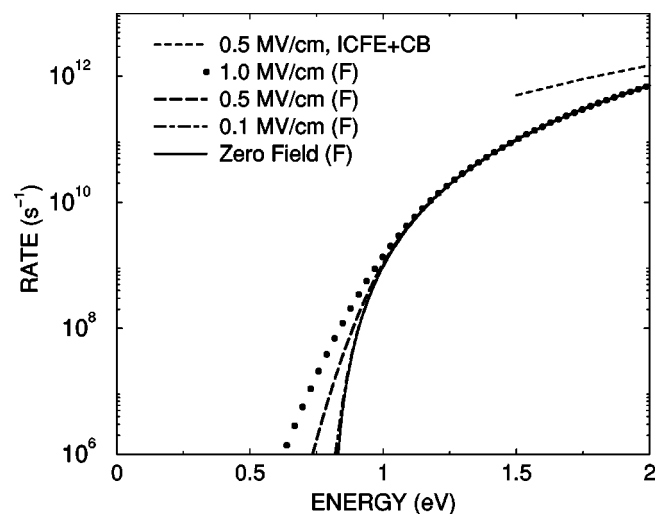

FIG. 3. Field dependent impact ionization rate for Si according to Eq. (37) where the full band structure is considered. Available results for $E \geqslant 1.5$ eV including the ICFE and collision broadening (see Ref. 10) (CB) are shown in addition (dashed line).
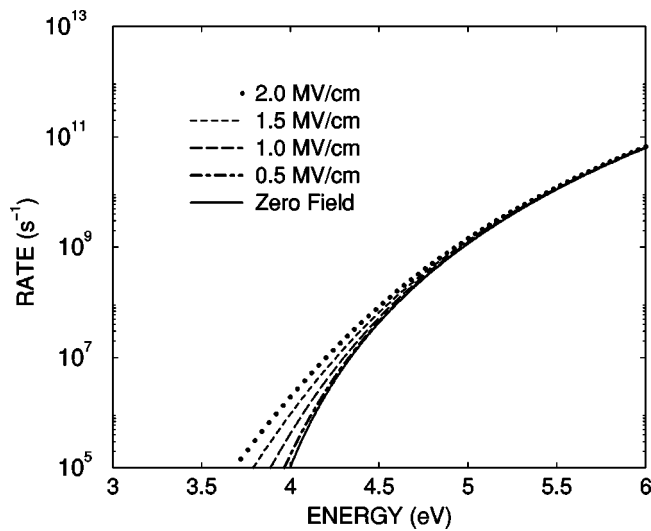
FIG. 4. Field dependent impact ionization rate for GaN according to Eq. (37).

FIG. 6. Same as Fig. 4 but for SrS.

The results for the field-dependent impact ionization rate in the wide band gap materials GaN, ZnS, and SrS are shown in Figs. 4–6. The behavior of ZnS and SrS is very similar, while the rate for GaN is substantially lower. This reflects the respective behavior of the zero-field rates.[7,8] The ICFE influences only the direct threshold region and leads to a systematic lowering of the threshold energy with increasing field strength. The sensitivity of this lowering is related to the effective masses which are introduced as material parameters in the quantity E_F^{ii} in Eq. (32) for the parabolic band result. The analytical form of Eq. (32) is also adapted for the fit formula (37) that reflects the full band structure via the parameter a and, again, the quantity E_F^{ii}. About 0.5 eV (1 eV) above the threshold energy, the impact ionization rate becomes already independent of the field for the narrow (wide) band gap materials.
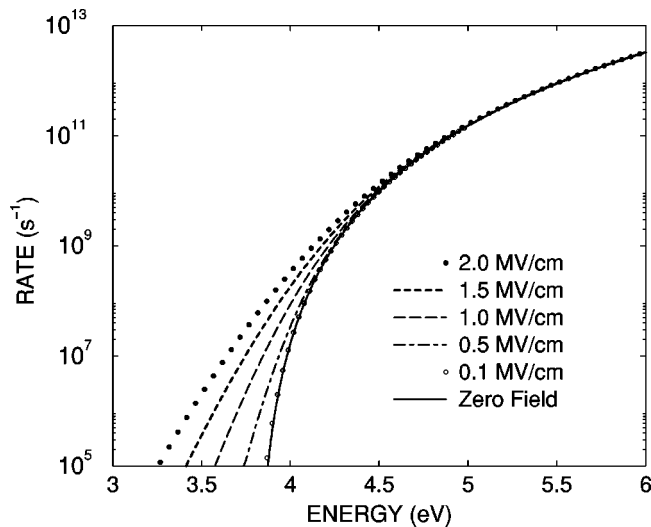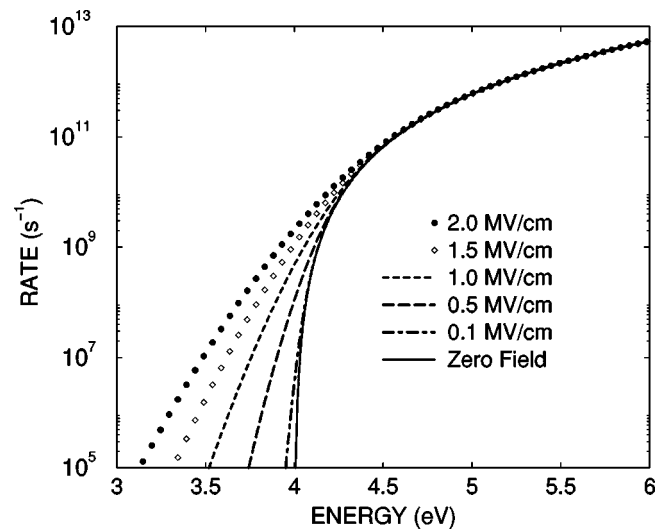
V. CONCLUSIONS

In this article, we have derived a field-dependent impact ionization rate, Eq. (29), based on a generalized quantum kinetic equation. We recover the analytical result (32) of Quade *et al.*[11] within the parabolic band approximation. Furthermore, we have proposed a fit formula, Eq. (37), that contains the influence of the full band structure via the parameter a and reproduces the numerical results for zero field strength.[4–8] We have evaluated Eq. (37) for arbitrary field strengths for a variety of semiconductor materials, see Figs. 2–6. The ICFE is of importance only in a narrow energy region around the threshold and leads to a lowering of the threshold energy.

The field-dependent impact ionization rate as given here can be used as input in Monte Carlo simulations of high-field electron transport. The consideration of the ICFE will lead to a modified EDF so that, e.g., the field dependence of the macroscopic ionization coefficient α_i as found experimentally for ZnS[34] can be studied in more detail.

Further effects such as collision broadening or the field dependence of the Wigner distribution function in Eq. (29) have to be considered in a self-consistent approach to the field effects. For instance, collision broadening can be incorporated in the present approach by replacing the one-particle energies E_p by quasiparticle energies ε_p. For this, an approximation for the self-energy is needed which leads to a broadened spectral function.

Another important effect for high field transport is dynamic screening. In principle, the Coulomb matrix element Eq. (30) for impact ionization has to be evaluated considering a wave vector and frequency dependent dielectric function $\varepsilon(q,\omega)$ instead of a statically screened one. This requires a complete numerical evaluation of the collision integral (29). The influence of dynamic screening on the impact ionization rate has been studied for the zero-field case for Si[35] and GaAs.[36] Comparing with our respective results for zero field strengths,[3] where a wave vector dependent dielectric function[37] has been used for the evaluation of the

FIG. 5. Same as Fig. 4 but for ZnS.

impact ionization matrix element, only minor differences have to be stated.

[1] A. P. Jauho, in *Quantum Transport in Semiconductors*, edited by D. K. Ferry and C. Jacoboni (Plenum, New York, 1992), p. 141.
[2] W. M. Ang, S. S. Pennathur, L. Pham, J. F. Wager, S. M. Goodnick, and A. A. Douglas, J. Appl. Phys. **77**, 2719 (1995).
[3] M. Stobbe, R. Redmer, and W. Schattke, Phys. Rev. B **49**, 4494 (1994).
[4] M. Reigrotzki, M. Stobbe, R. Redmer, and W. Schattke, Phys. Rev. B **52**, 1456 (1995).
[5] M. Reigrotzki *et al.*, J. Appl. Phys. **80**, 5054 (1996).
[6] M. Dür, S. M. Goodnick, S. S. Pennathur, J. F. Wager, M. Reigrotzki, and R. Redmer, J. Appl. Phys. **83**, 3176 (1998).
[7] M. Reigrotzki, M. Dür, W. Schattke, N. Fitzer, R. Redmer, and S. M. Goodnick, Phys. Status Solidi B **204**, 528 (1997).
[8] M. Dür, S. M. Goodnick, R. Redmer, M. Reigrotzki, M. Städele, and P. Vogl, J. Soc. Inf. Disp. (in press).
[9] J. R. Barker and D. K. Ferry, Phys. Rev. Lett. **42**, 1779 (1979); see also D. K. Ferry, *Semiconductors* (Macmillan, New York, 1991), Chap. 15.
[10] J. Bude, K. Hess, and G. J. Iafrate, Phys. Rev. B **45**, 10958 (1992).
[11] W. Quade, E. Schöll, F. Rossi, and C. Jacoboni, Phys. Rev. B **50**, 7398 (1994).
[12] L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (Benjamin, New York, 1962).
[13] A. P. Jauho and J. W. Wilkins, Phys. Rev. B **29**, 1919 (1984).
[14] S. K. Sarker, Phys. Rev. B **32**, 743 (1985).
[15] I. B. Levinson, Zh. Eksp. Teor. Fiz. **47**, 660 (1969) [Sov. Phys. JETP **30**, 362 (1970)].
[16] P. Lipavsky, F. S. Khan, F. Abdosalami, and J. W. Wilkins, Phys. Rev. B **43**, 4885 (1991).
[17] R. Bertoncini and A. P. Jauho, Phys. Rev. Lett. **68**, 2826 (1992).
[18] J. Y. Ryu and S. D. Choi, Phys. Rev. B **44**, 11 328 (1991).
[19] D. N. Zubarev, *Nonequilibrium Statistical Thermodynamics* (Consultants Bureau, New York, 1974).
[20] D. Y. Xing and C. S. Ting, Phys. Rev. B **35**, 3971 (1987).
[21] D. Y. Xing, P. Hu, and C. S. Ting, Phys. Rev. B **35**, 6379 (1987).
[22] L. V. Keldysh, Zh. Eksp. Teor. Fiz. **37**, 713 (1959) [Sov. Phys. JETP **37**, 509 (1960)].
[23] D. N. Zubarev, V. Morozov, and G. Röpke, *Statistical Mechanics of Non-equilibrium Processes, Vol. 1: Basic Concepts, Kinetic Theory* (Akademie-Verlag, Berlin, 1996).
[24] B. Robertson, Phys. Rev. **144**, 151 (1966).
[25] R. Kh. Amirov, S. A. Smolyanskii, and L. Sh. Shekhter, Teor. Mat. Fiz. **21**, 247 (1974).
[26] S. V. Peletminsky and A. A. Yatsenko, Zh. Éksp. Teor. Fiz. **53**, 1327 (1967) [Sov. Phys. JETP **26**, 773 (1967)].
[27] L. A. Pokrovsky, Dokl. Akad. Nauk SSSR **177**, 1054 (1967) [Sov. Phys. Dokl. **12**, 1135 (1968)]; **183**, 806 (1968) [**13**, 1216 (1969)].
[28] N. Sano and A. Yoshii, Phys. Rev. B **45**, 4171 (1992).
[29] J. Kolnik, I. H. Oguzman, K. F. Brennan, R. Wang, and P. P. Ruden, J. Appl. Phys. **79**, 8838 (1996).
[30] I. H. Oguzman, E. Bellotti, K. F. Brennan, J. Kolnik, R. Wang, and P. P. Ruden, J. Appl. Phys. **81**, 7827 (1997).
[31] E. Bellotti, B. K. Doshi, K. F. Brennan, J. D. Albrecht, and P. P. Ruden, J. Appl. Phys. **85**, 916 (1999).
[32] M. V. Fischetti and S. E. Laux, Phys. Rev. B **38**, 9721 (1988).
[33] M. Reigrotzki, Ph.D. thesis, University of Rostock, 1998.
[34] T. D. Thompson and J. W. Allen, J. Phys. C **20**, L499 (1987).
[35] Y. Kamakura, H. Mizuno, M. Yamaji, M. Morifuji, K. Taniguchi, and C. Hamaguchi, J. Appl. Phys. **75**, 3500 (1994).
[36] H. K. Jung, K. Taniguchi, and C. Hamaguchi, J. Appl. Phys. **79**, 2473 (1996).
[37] H. Nara and A. Morita, J. Phys. Soc. Jpn. **21**, 1852 (1966).