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Impact ionization rates of semiconductors in an electric field: The effect of collisional broadening

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A gauge invariant quantum kinetic equation which includes impact ionization, intracollisional field effect, and collisional broadening is derived in the frame of nonequilibrium Green's functions. We obtain analytical expressions for the impact ionization rate. For the wide band gap material ZnS, a substantial increase of the rate due to collisional broadening is obtained for moderate field strengths $\mathbf{E} \leqslant 500\,\mathrm{kV/cm}$. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1381554]

I. INTRODUCTION

The study of electron transport in wide band gap semiconductors at high electric fields is of great theoretical and practical interest.[1] Of particular relevance is the impact ionization rate—electron interband transitions caused by Coulomb collisions, since this is the dominant transport process in the high field domain.

The impact ionization rate was calculated by Keldysh[2] who performed an expansion of the energy around the ionization threshold using parabolic bands at zero electric field including Coulomb interaction in a momentum-independent approximation assuming constant matrix elements. Previous calculations for Si and GaAs,[3,4] ZnS,[5–7] SrS,[8] GaN,[8–11] InN,[12] and SiC,[13] again neglecting the field influence during the collision, have shown that the entire band structure in the Brillouin zone has to be considered when numerically evaluating the corresponding matrix element including direct, exchange, and umklapp processes. Pronounced contributions arise from higher conduction bands, especially in wide band gap materials like ZnS, GaN, or SrS.

Quade *et al.*[14] used a density matrix method to study electron transport with a finite electric field included in the collision process and a parabolic band approximation. They presented an analytical result for the field-dependent impact ionization rate which shows a lowering of the ionization threshold compared to the zero field case. Comparing these results with those using realistic band structures but neglecting the field, a field-dependent fit formula for the impact ionization rate was proposed recently.[15]

In the articles mentioned earlier, collisional broadening has been neglected. The broadening of one-particle energies $\varepsilon(\mathbf{p})$ due to two-particle collisions, see, e.g., Refs. 16 and 17, leads to an increase of the number of energetic electrons which should influence the rate of interband transitions. This has been shown for Si[18] solving the Barker–Ferry kinetic equation with a spectral function of Lorentzian shape. However, simple approximations such as the replacement of sharp electron spectral functions by broadened ones with a phenomenological width γ of, e.g., Lorentzian shape, $\delta(\hbar\omega-\varepsilon)\rightarrow 2\gamma/[(\hbar\omega-\varepsilon)^2+\gamma^2]$, have been found to be inadequate, as they violate energy conservation.[19] Fully consistent results for the spectral function can only be obtained from a solution of the two-time Kadanoff–Baym equations[20,21,16,19,22] which can be used as the starting point to construct proper broadened spectral functions (which turn out to be of essentially non-Lorentzian form, see later). This has been successfully demonstrated for electron-phonon scattering[23,24] and electron–electron scattering[25,26] in bulk semiconductors.

In the present article, we apply this idea to the computation of improved impact ionization rates which include collisional broadening via non-Lorentzian electron spectral functions. As expected, the energy broadening leads to a lowering of the ionization threshold which turns out to be significant for field-free systems and for not too strong static fields. For fields in the MV/cm range, the enhancement of the rates due to the field becomes the dominant process.

The outline of this article is as follows. In Sec. II, we present a gauge-invariant derivation of the quantum kinetic equation for semiconductors in an external time-dependent electrical field which selfconsistently includes impact ionization, the intracollisional field effect and collisional broadening. The derivation essentially follows recent work[27–29] and extends it to include collisional broadening and an arbitrary band structure $\varepsilon(\mathbf{p})$. In Sec. III, we consider the special case of a homogeneous field and calculate the impact ionization rate with collisional broadening included. Essentially analytical results can be given within the parabolic band approximation which straightforwardly extend previous results.[14,15] Numerical results for the impact ionization rate are presented in Sec. IV for ZnS. We propose a fit formula which takes into account the actual band structure, the intracollisional field effect, and collisional broadening. Conclusions are given in Sec. V.

II. GAUGE-INVARIANT DERIVATION OF THE QUANTUM KINETIC EQUATION

The transport properties of quantum systems can be described using the method of nonequilibrium Green's functions. The nonequilibrium state is given by the two-time correlation functions[16,17,20,30]

$$g_a^>(1,1')=\frac{1}{i\hbar}\langle\psi_a(1)\psi_a^\dagger(1')\rangle; \tag{1}$$

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$$g_a^<(1,1')=-\frac{1}{i\hbar}\langle\psi_a^\dagger(1')\psi_a(1)\rangle,$$

where $1\equiv(\mathbf{r}_1,t_1)$; $\psi^\dagger(\psi)$ are creation (annihilation) operators, and a labels the particle or quasiparticle species. The two-time functions $g^{\gtrless}$ are generalizations of the one-particle distribution function (density matrix) *f*, which follows from the time-diagonal element of $g^<$, $f_a(\mathbf{r}_1,\mathbf{r}_1',t)=-i\hbar g_a^<(1,1')|_{t_1=t_1'}$. In addition, the behavior of $g^{\gtrless}$ away from the time-diagonal characterizes the dynamic properties, such as the lifetime (width) of single-particle states.

A. Kinetic equation

The time evolution of the correlation functions in the presence of a homogeneous electrical field is given by the Kadanoff–Baym equations[20,31]

$$s_a(1)g_a^{\gtrless}(1,1')=\int d1''[\Sigma_a^R(1,1'')g_a^{\gtrless}(1'',1')+\Sigma_a^{\gtrless}(1,1'')g_a^A(1'',1')], \tag{2}$$

$$s_a(1)g_a^{R/A}(1,1')=\delta(1-1')+\int d1''\Sigma_a^{R/A}(1,1'')g_a^{R/A}(1'',1'), \tag{3}$$

to be supplemented by the adjoint equations, see, e.g., Ref. 22. Here g^R and g^A are the retarded and advanced Green's functions which are related to the correlation functions by $g_a^{R/A}(1,1')=\pm\Theta[\pm(t_1-t_1')][g_a^>(1,1')-g_a^<(1,1')]$. In Eqs. (2) and (3), s denotes the Schrödinger operator, $s_a(1)=i\hbar(\partial/\partial t_1)-\varepsilon_a(\mathbf{p}_1)-\Sigma^{\mathrm{HF}}(1)$, where $\mathbf{p}_1=(\hbar/i)\nabla_{\mathbf{r}_1}-(q_a/c)\mathbf{A}(\mathbf{r}_1,t_1)$, ε_a is the single-particle dispersion and Σ^{HF} the Hartree–Fock mean field. $\Sigma_a^{\gtrless}$ are the correlation parts of the selfenergy and $\Sigma_a^{R/A}(1,1')=\pm\Theta[\pm(t_1-t_1')]\times[\Sigma_a^>(1,1')-\Sigma_a^<(1,1')]$. The electrical field is represented by the vector potential $\mathbf{A}$ which is related to the field strength by $\mathbf{A}=-c\int_{-\infty}^t d\bar{t}\mathbf{E}(\bar{t})$, whereas the scalar potential is zero (vector potential gauge).

Our goal is a quantum kinetic equation for the Wigner function $f_a(\mathbf{k},t)$, which follows from the difference of the time-diagonal Eq. (2) for $g_a^<$ and its adjoint. To this end, we introduce center of mass and relative space and time variables, $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_{1'}$; $\mathbf{R}=(\mathbf{r}_1+\mathbf{r}_{1'})/2$; $\tau=t_1-t_{1'}$; $t=(t_1+t_{1'})/2$, and use $f_a(\mathbf{k},t)=-i\hbar g_a^<(\mathbf{k},\tau=0,t)$. The resulting equation has to be transformed to momentum space for which it is advantageous to use the gauge-invariant Fourier transform[17,27]

$$g_a(\mathbf{k},\tau,t)=\int d^3r\exp\left[-i\mathbf{r}\left(\mathbf{k}+\frac{q_a}{c}\int_{t-1/2\tau}^{t+1/2\tau}du\frac{\mathbf{A}(u)}{\tau}\right)\right]\times g_a(\mathbf{r},\tau,t), \tag{4}$$

and a straightforward calculation yields the gauge-invariant quantum kinetic equation[27,28]

$$\left[\frac{\partial}{\partial t}+q_a\mathbf{E}(t)\frac{\partial}{\partial\mathbf{k}_a}\right]f_a(\mathbf{k}_a,t)=2\,\mathrm{Re}\int_{t_0}^t dt''[g_a^>(\mathbf{k}_1,\tau_1,T_1)\Sigma_a^<(\mathbf{k}_1,-\tau_1,T_1)-g_a^<(\mathbf{k}_1,\tau_1,T_1)\Sigma_a^>(\mathbf{k}_1,-\tau_1,T_1)], \tag{5}$$

with

$$\mathbf{k}_1\equiv\mathbf{k}_a+\frac{q_a}{c}\mathbf{A}(t)-\frac{q_a}{c}\int_{t''}^t du\frac{\mathbf{A}(u)}{t-t''};\quad \tau_1\equiv t-t'';\quad T_1\equiv\frac{t+t''}{2}. \tag{6}$$

The lower integration limit t_0 is the initial time where the system is assumed to be uncorrelated.[32]

In the collision integrals [right-hand side (rhs)] of Eq. (5), we will use selfenergies in direct second order Born approximation, for which the gauge-invariant result is[27]

$$\Sigma_a^{\gtrless}(\mathbf{k}_a,\tau,t)=(i\hbar)^2\sum_b\int\frac{d\mathbf{k}_a'd\mathbf{k}_b'd\mathbf{k}_b}{(2\pi\hbar)^9}V_{ab}^2(\mathbf{k}_a-\mathbf{k}_a')\times(2\pi\hbar)^3\delta(\mathbf{k}_a+\mathbf{k}_b-\mathbf{k}_a'-\mathbf{k}_b')\times g_a^{\gtrless}(\mathbf{k}_a,\tau,t)g_b^{\gtrless}(\mathbf{k}_b',\tau,t)g_b^{\gtrless}(\mathbf{k}_b,-\tau,t), \tag{7}$$

where $V_{ab}(\mathbf{k}_a)$ is the Fourier transform of the statically screened Coulomb potential, and b in the sum runs over all species (bands or subbands) that interact with the chosen one (a). Inserting Eq. (7) into Eq. (5) we obtain the explicit quantum kinetic equation

$$\left[\frac{\partial}{\partial t}+q_a\mathbf{E}(t)\frac{\partial}{\partial\mathbf{k}_a}\right]f_a(\mathbf{k}_a,t)=2\hbar^2\,\mathrm{Re}\sum_b\int_{t_0}^t dt''\int\frac{d\mathbf{k}_a'd\mathbf{k}_b'd\mathbf{k}_b}{(2\pi\hbar)^6}\delta(\mathbf{k}_1+\mathbf{k}_b-\mathbf{k}_a'-\mathbf{k}_b')V_{ab}^2(\mathbf{k}_1-\mathbf{k}_a')[g_a^<(\mathbf{k}_1,\tau_1,T_1)\times g_a^>(\mathbf{k}_a,-\tau_1,T_1)g_b^>(\mathbf{k}_b',-\tau_1,T_1)g_b^<(\mathbf{k}_b,\tau_1,T_1)-g_a^>(\mathbf{k}_1,\tau_1,T_1)g_a^<(\mathbf{k}_a,-\tau_1,T_1)\times g_b^<(\mathbf{k}_b',-\tau_1,T_1)g_b^>(\mathbf{k}_b,\tau_1,T_1)]. \tag{8}$$

B. Generalized Kadanoff–Baym ansatz. Collisional broadening

In order obtain a closed equation for the Wigner function f_a, we have to express on the right-hand side of Eq. (8) the correlation functions $g^{\gtrless}$ also in terms of f and the electric field. This can be done only approximately. For nonequilibrium systems, the appropriate choice has been found to be the generalized Kadanoff–Baym ansatz[33] the gauge invariant version of which is given by[17,27]

$$g_a^{<}(\mathbf{k}_a,\tau,T) = -\frac{1}{i\hbar}\mathcal{A}_a(\mathbf{k}_a,\tau,T) f_a\left(\mathbf{k}_a(|\tau|,T), T-\frac{|\tau|}{2}\right), \tag{9}$$

$$g_a^{>}(\mathbf{k}_a,\tau,T) = \frac{1}{i\hbar}\mathcal{A}_a(\mathbf{k}_a,\tau,T)\left[1 - f_a\left(\mathbf{k}_a(|\tau|,T), T-\frac{|\tau|}{2}\right)\right], \tag{10}$$

where the spectral function $\mathcal{A}$ is defined by $\mathcal{A}_a(1,1') \equiv i\hbar[g_a^R(1,1') - g_a^A(1,1')]$, and

$$\mathbf{k}_a(\tau,T) = \mathbf{k}_a + \frac{q_a}{c}\int_{-1/2}^{1/2} du \int_{T-1/2\tau}^{T+u\tau} du' \mathbf{E}(u').$$

The spectral function follows from the solution of Eq. (3) which, however, again contains the two-time functions $g^{\gtrless}$ on the rhs. The simplest approximation is to neglect the rhs, i.e., to use the uncorrelated spectral function but still retain the full field in Eq. (3):[17,27]

$$\mathcal{A}_a^{\text{free}}(\mathbf{k},\tau,T) = \exp\left[\frac{1}{i\hbar}\int_{T-1/2\tau}^{T+1/2\tau} du\, \varepsilon_a\left(\mathbf{k} - \frac{q_a}{c}\mathbf{A}(u) + \frac{q_a}{c}\int_{T-1/2\tau}^{T+1/2\tau} du' \frac{\mathbf{A}(u')}{\tau}\right)\right]. \tag{11}$$

From comparison with full two-time calculations it is known that, in fact, exact inclusion of the field in the free propagators is crucial[34] and, if correlations are not strong, an approximate treatment of the latter is possible. Since we are interested in high-field transport in weakly correlated semiconductors, this treatment should be applicable.

The effect of correlations among the carriers is to introduce a damping of the spectral function away from the time diagonal, i.e., with increasing $|\tau|$. The simplest approximation is to replace $A^{\text{free}} \to A^{\text{free}} \exp(-\gamma|\tau|)$. In frequency space, this exponential damping yields a Lorentz line, but it was found to decay too slowly for $|\omega| \to \infty$ leading to a strong violation of total energy conservation.[19,25] Moreover, in this case no equilibrium solution of the kinetic equation is reached. The reason is the finite slope of $\exp(-\gamma|\tau|)$ at $\tau = 0$ which is in contrast to the zero slope found in full two-time calculations,[22,23,25,26] see Fig. 2 later. Haug *et al.*[23] proposed a simple nonexponential approximation which overcomes this problem and which was successfully applied to semiconductors with electron-phonon[23,24] and electron–electron scattering.[25,26] We will use this approximation to incorporate damping and collisional broadening effects in the spectral function (11):

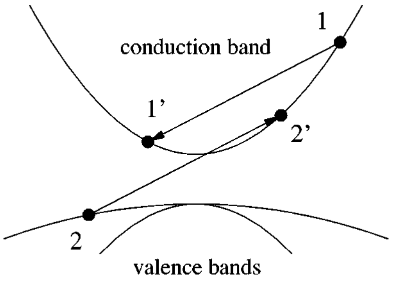

FIG. 1. Schematic impact ionization process for electrons.

$$\mathcal{A}_a(\mathbf{k},\tau,T) = \frac{1}{\cosh^{\alpha_0}(\omega_0\tau)}\mathcal{A}_a^{\text{free}}(\mathbf{k},\tau,T). \tag{12}$$

This approximation has a zero slope at $\tau = 0$, shows the correct exponential decay at large $|\tau|$, and an improved energy conservation behavior.[25,26] The two parameters α_0 and ω_0 are fit parameters. For electron–electron scattering, the natural decay time of the spectral function is the inverse plasma frequency, suggesting to use[15,25] $\omega_0 = \omega_{p1}$. This leaves open a single parameter. To obtain accurate results for α_0 we have performed solutions of the two-time Kadanoff–Baym Eqs. (2) and (3) for a field-free system. α_0 is fixed by the best fit of approximation (12) to the decay of the numerically obtained spectral function, see later.

Introducing this result for the damped spectral functions into Eq. (8), we obtain the gauge invariant quantum kinetic equation including the intracollisional field effect and collisional broadening

$$\begin{aligned}\left[\frac{\partial}{\partial t} + q_a\mathbf{E}(t)\frac{\partial}{\partial \mathbf{k}_a}\right] f_a(\mathbf{k}_a,t) = {} & \frac{2}{\hbar^2}\sum_b \int_{t_0}^{t} dt' \int \frac{d\overline{\mathbf{k}}_a d\overline{\mathbf{k}}_b d\mathbf{k}_b}{(2\pi\hbar)^6} |V(\mathbf{k}_a - \overline{\mathbf{k}}_a)|^2 \delta(\mathbf{k}_a + \mathbf{k}_b - \overline{\mathbf{k}}_a - \overline{\mathbf{k}}_b) \frac{1}{\cosh^{4\alpha_0}[\omega_0(t-t')]} \\ & \times \cos\left[\int_0^{t-t'} dt'' \Omega_{ab}(t'')\right] \{ f_a(\mathbf{k}_a + \Delta\mathbf{k}_a, t') f_b(\mathbf{k}_b + \Delta\mathbf{k}_b, t')[1 - f_a(\overline{\mathbf{k}}_a + \Delta\mathbf{k}_a, t')] \\ & \times [1 - f_b(\overline{\mathbf{k}}_b + \Delta\mathbf{k}_b, t')] - [1 - f_a(\mathbf{k}_a + \Delta\mathbf{k}_a, t')][1 - f_b(\mathbf{k}_b + \Delta\mathbf{k}_b, t')] f_a(\overline{\mathbf{k}}_a + \Delta\mathbf{k}_a, t') \\ & \times f_b(\overline{\mathbf{k}}_b + \Delta\mathbf{k}_b, t')\},\end{aligned} \tag{13}$$

where the frequencies Ω_{ab} are given by

$$\hbar\Omega_{ab}(t'') = \varepsilon_a(\mathbf{k}_a + \overline{\Delta\mathbf{k}_a}) + \varepsilon_b(\mathbf{k}_b + \overline{\Delta\mathbf{k}_b}) - \varepsilon_a(\overline{\mathbf{k}}_a + \overline{\Delta\mathbf{k}_a}) - \varepsilon_b(\overline{\mathbf{k}}_b + \overline{\Delta\mathbf{k}_b}). \tag{14}$$

The field leads to a drift of the band energies ε_a as well as to a shift of the arguments of the populations f_a (intracollisional field effect). The corresponding momentum shifts are given by $\overline{\Delta\mathbf{k}_a} \equiv q_a[\mathbf{A}(t) - \mathbf{A}(t-t'')]/c$ and $\Delta\mathbf{k}_a \equiv q_a[\mathbf{A}(t) - \mathbf{A}(t')]/c$, which are just the momentum gain of particle a in the electric field during the time interval $[t-t'', t]$ and $[t', t]$, respectively.

III. SEMICONDUCTOR IN A HOMOGENEOUS ELECTRIC FIELD

After having derived a gauge invariant quantum kinetic equation we will now treat electron transport in semiconductors at high electric field strengths. We consider a constant homogeneous external electrical field E_0 which yields $\mathbf{A}(t)=-c\mathbf{E}_0 t$. For the momentum shifts follows $\overline{\Delta\mathbf{k}_a}=-q_a\mathbf{E}_0 t''$ and $\Delta\mathbf{k}_a=-q_a\mathbf{E}_0(t-t')$.

A. Impact ionization rate

The electron–electron collision integral is studied in more detail. We are especially interested in the inelastic process of impact ionization which has a strong influence on the electron distribution function at high electric field strengths: A conduction band electron impact ionizes a valence band electron, i.e., $1+2\rightarrow\overline{1}+\overline{2}$, see Fig. 1.

The respective field-dependent collision integral $J_{ee}^{(ii)}$ with broadening effects follows immediately from Eq. (13) and is given by

$$J_{ee}^{ii}(\mathbf{k}_a,\mathbf{E}_0,t)=\frac{2}{\hbar^2}\int_{t_0}^{t}dt'\int\frac{d\overline{\mathbf{k}}_a d\overline{\mathbf{k}}_b d\mathbf{k}_b}{(2\pi\hbar)^6}|V(\mathbf{k}_a-\overline{\mathbf{k}}_a)|^2\delta(\mathbf{k}_a+\mathbf{k}_b-\overline{\mathbf{k}}_a-\overline{\mathbf{k}}_b)\frac{1}{\cosh^{4\alpha_0}[\omega_0(t-t')]}$$
$$\times\cos\left[\int_0^{t-t'}dt''\Omega(t'')\right](f_a[\mathbf{k}_a(t-t'),t']f_b[\mathbf{k}_b(t-t'),t']\{1-f_a[\overline{\mathbf{k}}_a(t-t'),t']\}\{1-f_b[\overline{\mathbf{k}}_b(t-t'),t']\}$$
$$-\{1-f_a[\mathbf{k}_a(t-t'),t']\}\{1-f_b[\mathbf{k}_b(t-t'),t']\}f_a[\overline{\mathbf{k}}_a(t-t'),t']f_b[\mathbf{k}_b(t-t'),t']), \tag{15}$$

where $\hbar\Omega(t)=\varepsilon_c[\mathbf{k}_a(t)]+\varepsilon_v[\mathbf{k}_b(t)]-\varepsilon_c[\overline{\mathbf{k}}_a(t)]-\varepsilon_c[\overline{\mathbf{k}}_b(t)]$ and $\mathbf{k}_a(t)=\mathbf{k}_a-e\mathbf{E}_0 t$. The momentum $\mathbf{k}_b$ runs over the valence bands and $\mathbf{k}_a$, $\overline{\mathbf{k}}_a$ and $\overline{\mathbf{k}}_b$ over the conduction bands, respectively.

Supposing that the semiconductor is not highly excited, the conduction bands are almost empty so that $(1-f_{\text{con}})\approx 1$ applies. Simultaneously, the valence bands are almost filled and we have $f_{\text{val}}\approx 1$. Then, the inscattering term (second term) in the square brackets in Eq. (15) which is proportional to the product of distribution functions of conduction band electrons can be neglected compared with the outscattering term (first term) in the balance for the population of states with momentum $\mathbf{k}_a$. Furthermore, we perform the long-time Markov limit, i.e., we take $t'\rightarrow t$ in the arguments of the momenta and $t_0\rightarrow-\infty$. The collision integral for field-dependent impact ionization can then be represented as

$$J_{ee}^{ii}(\mathbf{k}_a,\mathbf{E}_0,t)=r^{ii}(\mathbf{k}_a,\mathbf{E}_0)f_a(\mathbf{k}_a,t), \tag{16}$$

where the impact ionization rate is given by

$$r^{ii}(\mathbf{k}_a,\mathbf{E}_0)=\frac{2}{\hbar^2}\int_{-\infty}^{t}dt'\int\frac{d\overline{\mathbf{k}}_a d\overline{\mathbf{k}}_b d\mathbf{k}_b}{(2\pi\hbar)^6}|V(\mathbf{k}_a-\overline{\mathbf{k}}_a)|^2$$
$$\times\delta(\mathbf{k}_a+\mathbf{k}_b-\overline{\mathbf{k}}_a-\overline{\mathbf{k}}_b)$$
$$\times\frac{1}{\cosh^{4\alpha_0}[\omega_0(t-t')]}\cos\left[\int_0^{t-t'}dt''\Omega(t'')\right]. \tag{17}$$

B. Parabolic band approximation: Analytical results

We first evaluate Eq. (17) for a direct semiconductor with a fundamental gap energy E_g and spherical parabolic bands with effective masses m_v for the valence and m_c for the conduction band. We follow the notation given in Ref. 14 and define $\alpha=m_c/m_v$ and $\mu=(1+2\alpha)/(1+\alpha)$. We use a Debye-like statically screened Coulomb potential with an inverse screening length λ and overlap integrals F_{cc} and F_{cv} relevant for the impact ionization process[14]

$$V(\mathbf{q})=\frac{e^2|F_{cv}F_{cc}|}{\varepsilon\varepsilon_0 V_g}\frac{1}{|\mathbf{q}|^2+\lambda^2}, \tag{18}$$

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

Following the evaluation of Quade *et al.*,[14] an essentially analytical expression for the field-dependent impact ionization rate for an electron having a kinetic energy $E_{\mathbf{k}_a}=|\mathbf{k}_a|^2/2m_c$ can be derived

$$r^{ii}(E_{\mathbf{k}_a},E_0)$$
$$=\frac{1}{\tau_I}\int_0^\infty dE\left\{\frac{1}{2}\left[\sqrt{\frac{E_{\mathbf{k}_a}}{P(E_{\mathbf{k}_a},E)}}+\sqrt{\frac{P(E_{\mathbf{k}_a},E)}{E_{\mathbf{k}_a}}}\right]-1\right\}$$
$$\times\int_0^\infty dx\,\frac{1}{\pi}\cos\left(\frac{1}{3}x^3+\frac{E_{\text{th}}-E_{\mathbf{k}_a}+E}{E_F^{ii}}x\right)$$
$$\times\frac{1}{E_F^{ii}}\left[\cosh^{4\alpha_0}\left(\frac{\omega_0}{\omega_F^{ii}}x\right)\right]^{-1}. \tag{19}$$

$E_{\text{th}}=\mu E_g$ is the threshold energy for impact ionization. Further definitions are

$$P(E_{\mathbf{k}_a},E)=\tfrac{1}{2}\left[\sqrt{(E_\lambda-E_{\mathbf{k}_a}+E)^2+4E_\lambda E_{\mathbf{k}_a}}\right.$$
$$\left.-(E_\lambda-E_{\mathbf{k}_a}+E)\right],$$

$$E_\lambda = \frac{\hbar^2\lambda^2}{2m_c}, \quad E_F^{ii} = \mu\hbar\omega_F^{ii}, \quad \omega_F^{ii} = \left[\frac{(1+\alpha)(eE_0)^2}{8\hbar m_c}\right]^{1/3}, \tag{20}$$

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

The special case of a free spectral function follows trivially by setting $\alpha_0 = 0$, and we immediately recover previous results for the field-dependent impact ionization rate.[14,15]

IV. NUMERICAL RESULTS

We perform numerical calculations for the impact ionization rate, Eqs. (19) and (23), for the wide band gap semiconductor ZnS at room temperature $T = 300\,\mathrm{K}$ and also at $T = 200\,\mathrm{K}$. Its effective masses are $m_c = 0.456 m_0$ and $m_v = 0.178 m_0$.

A. Computation of the broadened spectral function

For the evaluation of the field-dependent impact ionization rate Eq. (19), the parameter α_0 in the spectral function which describes the influence of collisional broadening in this process has to be determined since the second parameter is fixed by $\omega_0 = \omega_{\mathrm{pl}}$. This broadening arises from all scattering mechanisms in the system, i.e., electron-phonon, electron-impurity, and elastic as well as inelastic electron–electron scattering. Here we assume that elastic carrier–carrier scattering is dominant, and neglect the other broadening mechanisms. Further, we assume that the external field does not alter the broadening qualitatively. In fact, elastic scattering rates in the presence of the field decrease with growing field strength,[35] and this assumption will not be correct in strong fields. However, as our calculations will show, broadening effects are of importance for the impact ionization rates only at weak fields—so this approximation is justified.

Thus, we solve the field-free Kadanoff–Baym equations for an electron-hole plasma with statically screened elastic Coulomb interaction, which yields an "exact" result for the spectral function $\mathcal{A}_a(\mathbf{k},\tau,T)$, for numerical details see Refs. 22 and 25. Using then Eq. (12) as an approximation to the numerical result, we vary α_0 until best agreement is achieved. The result for the absolute value of the numerical and fitted spectral functions is shown in Fig. 2 for an electron-hole plasma with a density $n = 10^{16}\,\mathrm{cm}^{-3}$ and a temperature $T = 300\,\mathrm{K}$. To eliminate the oscillations of the spectral function (it oscillates as a function of the relative time τ with the renormalized single-particle energy), it is convenient to plot the absolute value of $\mathcal{A}$. As one can see the fit reproduces the numerical result both for small and large τ rather well. Although there are small deviations in the central part of the curve, the 1/cosh function yields a good overall agreement which is achieved with a single fitting parameter α_0. Further, we find that the same value α_0 fits the spectral function almost equally well in the whole range of electron momenta. This can be seen by comparing the upper and lower figure parts which contain two limiting cases.

Finally, we confirm in the upper figure that a Lorentzian (exponential) spectral function cannot reproduce the numerical result for the decay of the spectral function. No matter how the damping coefficient in the exponential is chosen, no agreement is possible. In particular, the decay at $\tau = 0$ is much too strong which translates into much too high values of the Lorentzian spectral function at high frequencies. This fitting procedure was repeated for several densities n and temperatures T; in Fig. 3 $n = 10^{16}\,\mathrm{cm}^{-3}$ and $T = 300\,\mathrm{K}$, in Fig. 4 $n = 10^{16}\,\mathrm{cm}^{-3}$ and $T = 200\,\mathrm{K}$, and for Fig. 5 we have used $n = 10^{17}\,\mathrm{cm}^{-3}$ and $T = 300\,\mathrm{K}$ resulting $\alpha_0 = 28$, 14, and 2, respectively.

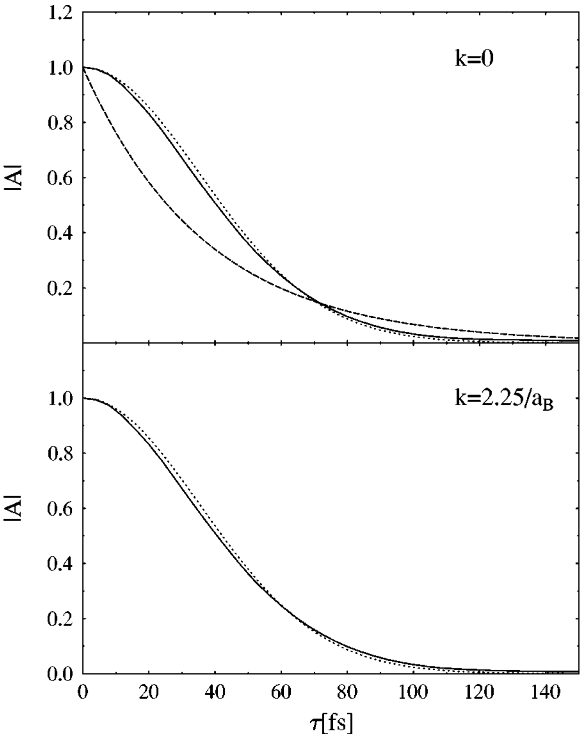

FIG. 2. Absolute value of the electron spectral function from solution of the field-free Kadanoff–Baym equations for the momentum $k = 0$ (upper fig.) and $k = 2.25/a_B$ (lower fig.). Full line—two-time Kadanoff–Baym result, dots—1/cosh approximation, dashes—exponential (Lorentzian) function. Density and temperature are $n = 10^{16}\,\mathrm{cm}^{-3}$ and $T = 300\,\mathrm{K}$. The obtained value for α_0 is 28, the plasma frequency $\omega_0 = 5.29\times 10^{12}\,\mathrm{s}^{-1}$.

B. Parabolic band approximation

In Fig. 3, we illustrate the influence of collisional broadening on the impact ionization rate in ZnS according to Eq. (19) within the parabolic band approximation. The intracollisional field effect alone (full lines with $\alpha_0 = 0$) yields a lowering of the threshold energy E_{th} which is proportional to the applied field. The impact ionization rate is increased only in a narrow energy region below 4.5 eV. Collision broadening leads to similar trends, i.e., a further lowering of the threshold energy and an increased rate in a narrow energy region above threshold. However, this effect is important for low fields whereas the ICFE dominates the behavior at high fields.

In Fig. 4, we show similar results for the impact ionization rate as in Fig. 3 but for a lower temperature of 200 K. There, fewer scattering events occur in the electron system and the spectral function is narrower compared with the case

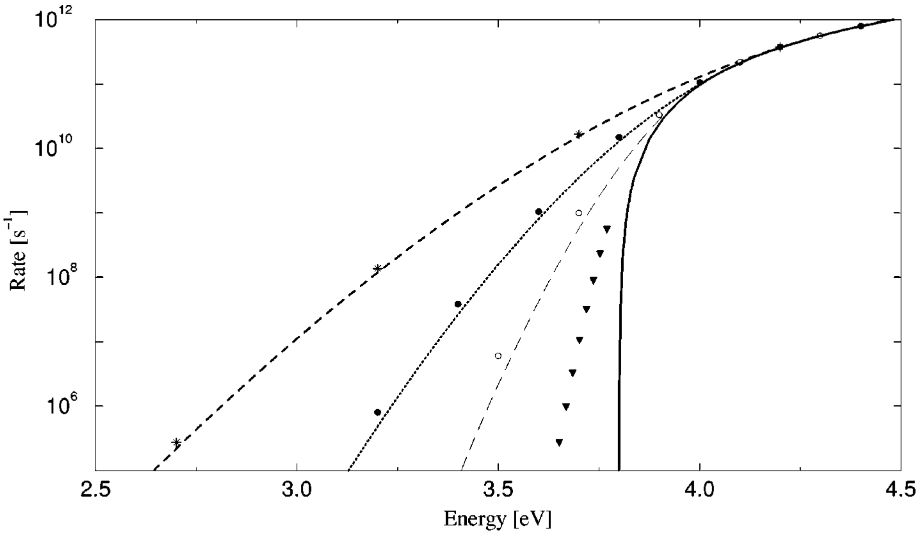

FIG. 3. Field dependent impact ionization rate for ZnS within the parabolic band approximation. Comparison with the case where collisional broadening effect is included. Density of carriers $n = 10^{16}\,\mathrm{cm}^{-3}$, temperature $T = 300\,\mathrm{K}$, and plasma frequency $\omega_0 = 5.29 \times 10^{12}\,\mathrm{s}^{-1}$. With $E_0 = 0$ MV/cm we have solid line for $\alpha_0 = 0$ and triangles for $\alpha_0 = 28$, for $E_0 = 0.5$ MV/cm long dashed line for $\alpha_0 = 0$ and empty cicles for $\alpha_0 = 28$, with $E_0 = 1.0$ MV/cm dotted line for $\alpha_0 = 0$ and solid circles for $\alpha_0 = 28$, with $E_0 = 2.0$ MV/cm dashed line for $\alpha_0 = 0$ and stars for $\alpha_0 = 28$.

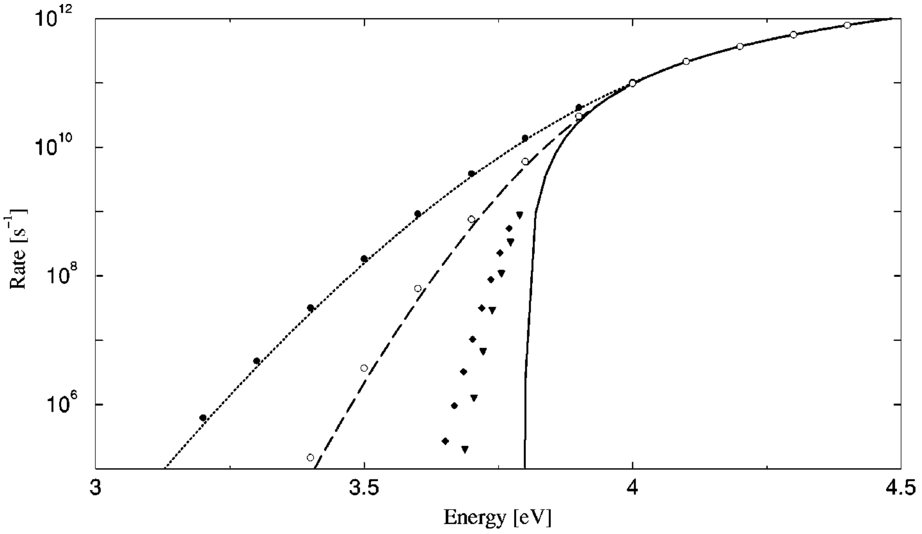

FIG. 4. Field dependent impact ionization rate for ZnS within the parabolic band approximation. Here $n = 10^{16}\,\mathrm{cm}^{-3}$, $T = 200\,\mathrm{K}$ and $\omega_0 = 5.29 \times 10^{12}\,\mathrm{s}^{-1}$. With $E_0 = 0$ MV/cm we have solid line for $\alpha_0 = 0$ and triangles for $\alpha_0 = 14$, for $E_0 = 0.5$ MV/cm long dashed line for $\alpha_0 = 0$ and empty circles for $\alpha_0 = 14$, with $E_0 = 1.0$ MV/cm dotted line for $\alpha_0 = 0$ and solid circles for $\alpha_0 = 14$. The diamonds here are those points in Fig. 3 denoted with triangles.

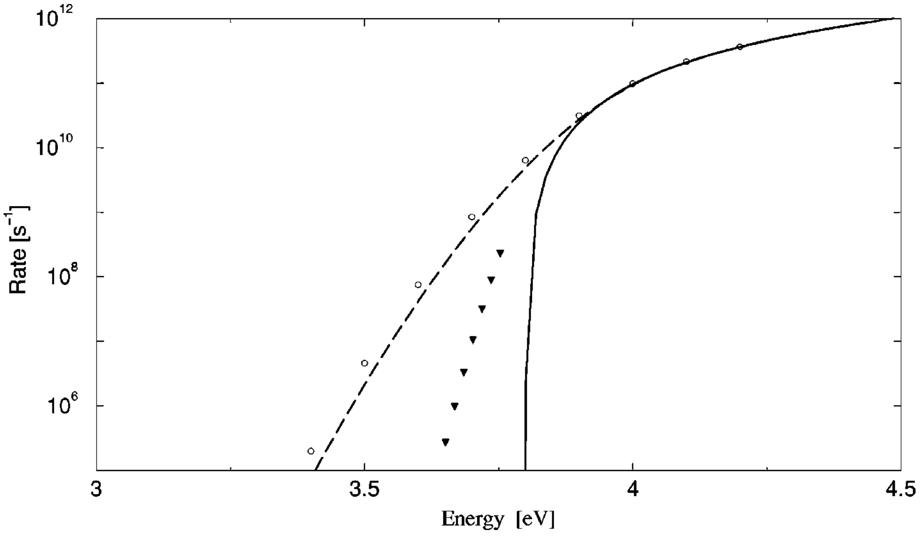

FIG. 5. Field dependent impact ionization rate for ZnS within the parabolic band approximation with $n = 10^{17}\,\mathrm{cm}^{-3}$, $T = 300\,\mathrm{K}$, and $\omega_0 = 16.75 \times 10^{12}\,\mathrm{s}^{-1}$. With $E_0 = 0$ MV/cm we have solid line for $\alpha_0 = 0$ and triangles for $\alpha_0 = 2$, for $E_0 = 0.5$ MV/cm long dashed line for $\alpha_0 = 0$ and empty circles for $\alpha_0 = 2$.

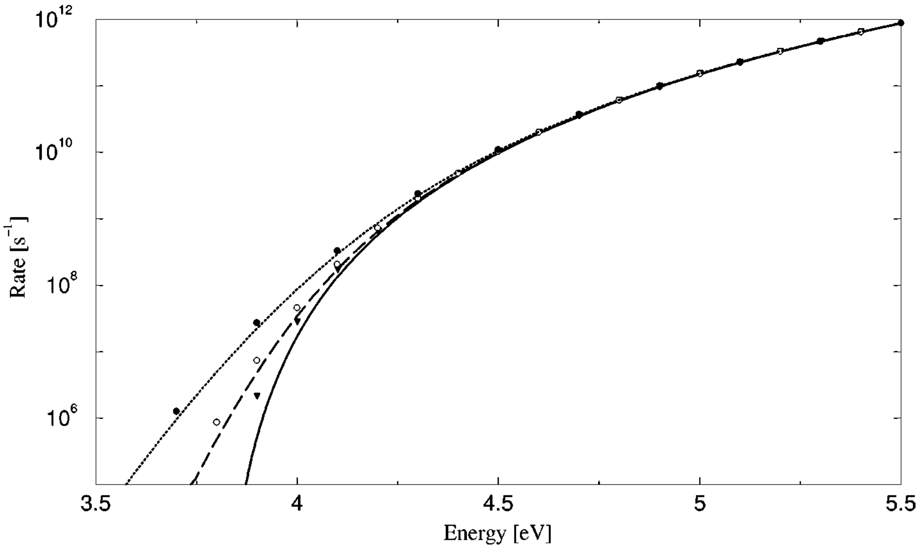

FIG. 6. Field dependent impact ionization rate for ZnS using the fit formula Eq. (23). The parameters are $n=10^{16}\,\mathrm{cm}^{-3}$, $T=300\,\mathrm{K}$, $\omega_0=5.29\times10^{12}\,\mathrm{s}^{-1}$, and $a=5.073$. With $E_0=0\,\mathrm{MV/cm}$ we have solid line for $\alpha_0=0$ and triangles for $\alpha_0=28$, with $E_0=0.5\,\mathrm{MV/cm}$ long dashed line for $\alpha_0=0$ and empty cicles for $\alpha_0=28$, with $E_0=1.0\,\mathrm{MV/cm}$ dotted line for $\alpha_0=0$ and solid circles for $\alpha_0=28$.

of 300 K and, thus, the influence of collisional broadening on the rate is weaker. The curves in diamonds (higher temperature) and triangles show it clearly.

Varying the carrier density has little effect on the rate which can be seen from Fig. 5 where we have taken $10^{17}\,\mathrm{cm}^{-3}$ instead of $10^{16}\,\mathrm{cm}^{-3}$ as in Fig. 3. The curve for low field strength (about one kV/cm) neglecting broadening effect coincide essentially with the curve for zero field neglecting collisional broadening in the cases of Fig. 3–6, what means the broadening effect is crucial in describing transition between valence and conduction band.

C. Realistic band structure

We have shown in previous articles[5–8] that 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. The numerical results for the field-independent impact ionization rate taking into account realistic band structures can be parameterized in terms of a generalized Keldysh formula according to

$$r^{ii}_{\rm Fit}(E_{\mathbf{k}},0)=C\left[\frac{E_{\mathbf{k}}-E_{\rm th}}{E_{\rm th}}\right]^a, \tag{21}$$

where the prefactor C, the threshold energy $E_{\rm th}$, and the power a were given for a variety of semiconductor materials. The parameters for ZnS are threshold energy $E_{\rm th}=3.8\,\mathrm{eV}$, and the actual band fit parameters $a=5.073$ and $C=5.935\,10^{10}\,\mathrm{eV}^{-a}$. The influence of the band structure manifests itself in values $a>2$, whereas $a=2$ in the original Keldysh formula derived for parabolic bands and constant matrix elements.

In order to derive a general result for the impact ionization rate which takes into account a realistic band structure as well as the field and broadening effects, we study various limiting cases as in the previous article.[15] Assuming constant matrix elements in Eq. (19) as Keldysh in his original article, i.e., replacing $|\mathbf{q}|^2+\lambda^2\rightarrow 2m_cE_{\rm th}/\hbar^2$, the following expression is obtained within the parabolic band approximation:

$$\begin{aligned} r^{ii}(E_k,E_0) &= \frac{1}{\tau_k}\int_0^\infty dE\left(\frac{E}{E_{\rm th}}\right)^2\int_0^\infty dx\,\frac{1}{\pi}\cos\left(\frac{1}{3}x^3+\frac{E_{\rm th}-E_k+E}{E_F^{ii}}x\right)\\ &\quad\times\frac{1}{E_F^{ii}}\left[\cosh^{4\alpha_0}\left(\frac{\omega_0}{\omega_F^{ii}}x\right)\right]^{-1},\\ \frac{1}{\tau_K} &= \frac{1}{32\pi^2(1+2\alpha)^{3/2}}\left(\frac{e^2F_{cc}F_{cv}\sqrt{m_c}}{\varepsilon\varepsilon_0\hbar^{3/2}}\right)^2. \end{aligned} \tag{22}$$

Performing the zero field limit, i.e., $E_F^{ii}\rightarrow 0$, and neglecting collisional broadening, i.e., $\alpha_0=0$, we obtain the original Keldysh result (21) with $a=2$. We propose a fit formula for the impact ionization rate that takes into account the influence of an applied electric field during the collision, the effects of a broadened spectral function, and a realistic band structure according to

$$\begin{aligned} r^{ii}(E_{\mathbf{k}},E_0) &= C\int_0^\infty dE\left(\frac{E}{E_{\rm th}}\right)^a\int_0^\infty dx\,\frac{1}{\pi}\cos\left(\frac{1}{3}x^3+\frac{E_{\rm th}-E_{\mathbf{k}}+E}{E_F^{ii}}x\right)\\ &\quad\times\frac{1}{E_F^{ii}}\left[\cosh^{4\alpha_0}\left(\frac{\omega_0}{\omega_F^{ii}}x\right)\right]^{-1}. \end{aligned} \tag{23}$$

Neglecting broadening effects, i.e., taking $\alpha_0=0$, we obtain our previous result.[15]

In Fig. 6, we compare the numerical results according to Eq. (23) for ZnS which include now the field effect, collisional broadening, and a realistic band structure as well. Collisional broadening is important for lower field strengths, whereas the field effect is naturally dominating the behavior of the impact ionization rate at high field strengths above 0.5 MV/cm.

V. CONCLUSIONS

We have derived a field-dependent impact ionization rate including the effects of collisional broadening, based on a gauge invariant quantum kinetic equation which was here derived considering a arbitrary band energy $\varepsilon(\mathbf{p})$, and using the frame of nonequilibrium Green's functions. We recover our previous, essentially analytical result[15] within the parabolic band approximation and neglecting collisional broadening. The latter is included using an appropriate parameterization for the one-particle spectral function as proposed by Haug and Banyai.[23] Furthermore, we propose a fit formula, Eq. (23), that contains the influence of a realistic band structure via the parameter a.

The numerical evaluation of Eqs. (19) and (23) for arbitrary field strengths is performed for the wide band gap semiconductor ZnS. The field and broadening effects are of importance only in a narrow energy region near the threshold and lead both to a lowering of the threshold energy. For low fields, the broadening effect is essential whereas the field effect becomes dominant at high fields. Although the presented treatment of collisional broadening is not selfconsistent (neglect of the field in the numerical spectral function and of other scattering mechanisms than elastic e-e scattering for the spectral function), we expect that it gives the correct result in the region of weak field where broadening is important. Moreover, this procedure may be generalized to other scattering mechanisms which will result in a modification of the parameters α_0 and ω_0.

The field-dependent impact ionization rate as given here can be used as input in Monte Carlo simulations of high-field electron transport. Then, the role of the intracollisional field and broadening effect in impact ionization processes and, consequently, their influence on the macroscopic ionization coefficient where indications for a nonlinear field-dependence have been found for ZnS,[36] can be studied in more detail.

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