Quantum theory of impact ionization in coherent high-field semiconductor transport

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Generation of carriers in semiconductors by impact ionization is studied under the influence of a constant, arbitrarily high electric field. Using the density-matrix approach a system of equations for the coherent dynamics of electrons and holes in the presence of impact ionization and Auger recombination is derived, which extends the semiconductor Bloch equations by the inclusion of impact-ionization density-correlation functions as additional dynamic variables. From these equations we recover the pure (Zener) and the photon-induced (Franz-Keldysh) carrier tunneling rate and derive an expression for the field-assisted impact-ionization scattering rate. Different levels of approximation of the kinetic equations are discussed. It is shown that in contrast to the semiclassical treatment in the presence of an electric field, a fixed impact-ionization threshold does no longer exist, and the impact-ionization scattering rate is drastically enhanced around the semiclassical threshold by the intracollisional field effect. The close connection of field-assisted impact ionization to the Franz-Keldysh effect is emphasized.

I. INTRODUCTION

In today's ultrasmall semiconductor devices carriers are subject to electric fields up to 10^6 V/cm. In this field regime carrier-generating processes such as impact ionization[1] and Zener ionization[2] influence the device behavior significantly. These processes are normally treated as independent ones and their relative importance is sometimes regarded to be distinguishable through a different dependence upon the lattice temperature.[3] In indirect semiconductors like silicon, Zener tunneling rates can often be explained only by considering phonon assistance[4] which allows for momentum conservation in an indirect transition from the valence band maximum to the conduction band minimum. As was already pointed out by Keldysh,[5] instead of phonons, also impact ionization can assist the Zener tunneling process which may equally well help to conserve momentum in indirect materials. His idea has already stimulated the work of Refs. 6–8 and is further developed here.

In an impact ionization process a high-energy conduction electron collides with a valence electron with the consequence that this latter electron is lifted from the valence to the conduction band. In an electron-hole picture, this process eventually leaves two electrons in the conduction band and a hole in the valence band. The role of impact ionization in semiconductor devices is particularly pronounced since this process (i) is autocatalytic, i.e., represents a positive feedback, and (ii) can be originated by electrons as well as by holes, which leads to the eventual destruction of the device by generating a coupled avalanche of both types of carriers.

The Zener process, on the other hand, describes the transition of a valence band electron into the conduction band without participation of other carriers and without change of momentum (if not assisted by other scattering processes). In contrast to impact ionization it is caused only by the external field and not by a carrier already in the conduction band. Zener transitions occur because the effect of the electric field in a semiconductor is composed of a vacuumlike (acceleration) and an isolated-atomlike (polarization) behavior. The first phenomenon leads to the intracollisional field effect for scattering processes.[9] The second one mixes states of different bands. Both effects together are involved in real Zener transitions.[10,11] The Zener process assisted by photons is called the Franz-Keldysh effect and gives a direct measurable evidence of the influence of an external electric field on the tunneling of carriers through the forbidden gap.

In general, for all types of scattering processes that change the number of particles within one band the intracollisional field effect is present as well and can supply energy to the carriers. This is especially true for impact ionization and, as we will show, leads to a softening of the impact-ionization threshold. This softening is of a fundamentally different nature than that which arises due to the band structure and which can be understood already in terms of semiclassical energy and crystal momentum conservation.[12,13]

Although the breakdown of the semiclassical theory of

impact ionization and the need for a full quantum mechanical treatment in the regime of ultrashort time and length scales in modern nanoelectronics is generally acknowledged, it is difficult to verify specific quantum mechanical effects directly in semiconductor experiments. This, for example, is true for effects concerning the role of energy-time uncertainty in scattering processes, but also for the effect of an electric field on coherent carrier-generation processes. With the availability of very efficient tunable femtosecond lasers and experimental setups such as four-wave mixing the situation has somewhat improved in the field of semiconductor optics.

In this paper, we develop a quantum transport theory of impact ionization which allows for a unified treatment of coherent high-field effects. In the theory we include the coherence of electron-hole pairs (interband polarization) and a homogeneous arbitrarily high electric field with both its polarizing and accelerating effects. We especially study its effect on the process of impact ionization and elaborate its close relation to the Franz-Keldysh effect. The fundamentals of the density-matrix approach that we adopt are presented in Sec. II. Here, we introduce our semiconductor model and derive an equation of motion for operators which includes the acceleration due to a homogeneous electric field through a time-dependent basis (accelerated Bloch waves). Differential equations for the electron and hole distribution functions, the interband polarization, and the impact-ionization density-correlation functions are obtained. In Sec. III, this hierarchy of equations, which couples to other higher-order correlation functions, is closed by a mean field approximation. By neglecting the impact-ionization density-correlation functions, in Sec. III A the semiconductor Bloch equations[14] for the electron and hole distribution functions and for the polarization are obtained in our accelerated basis. The coherent first-order contributions of impact ionization and Auger recombination here appear through a "self-energy" and an "internal field." Then in Sec. III B the full system of differential equations is derived including impact ionization (and Auger recombination) up to second order.

In the following two sections, the obtained system of dynamic equations is discussed. In Sec. IV A the semiconductor Bloch equations in the accelerated frame are used to derive the familiar expression for the Zener tunneling rate.[4,10,11] It is shown in Sec. IV B that the superposition of the constant external electric field and an oscillating light field leads from Zener tunneling to the Franz-Keldysh effect.[15] In Sec. V we examine carrier generation due to impact ionization and, for nondegenerate conditions, derive a formula for the total rate of change of electron concentration in the conduction band, which includes tunneling due to the electric field and can be regarded as an impact-ionization assisted tunneling or field-assisted impact ionization. This formula gives direct evidence of the close connection of impact ionization with the Franz-Keldysh effect. This connection was already noted in Ref. 16 where impact ionization in the presence of an electric field was called a two-particle Franz-Keldysh effect.

Finally, in Sec. VI we summarize our results and draw conclusions. Some technical calculations are given in the appendix.

II. PHYSICAL SYSTEM AND THEORETICAL APPROACH

In this section we introduce the Hamiltonian of the system and the basic quantities such as distribution functions, polarization, and two-particle correlation functions. Then differential equations for those basic quantities are derived from the Heisenberg equation of motion. It is shown that they do not only couple to each other but also to higher-order correlation functions. The latter ones are again coupled to correlation functions of even higher order. This infinite hierarchy of differential equations has to be truncated by some suitable approximation in order to obtain a closed set of equations. Such a procedure will be used in the following section.

A. The Hamiltonian

Our semiconductor model is given by the following two-band Hamiltonian:

$$H = H_0 + H_{\mathcal{E}} + H_1 , \tag{1}$$

where

$$H_0 = \sum_k E_c(k)\, c_k^\dagger c_k + \sum_k E_v(k)\, d_k^\dagger d_k \tag{2}$$

describes free electrons in the conduction band c and holes in the valence band v with energy dispersion relations $E_c(k)$ and $E_v(k)$, respectively. The mode operators $c_k^\dagger$, c_k and $d_k^\dagger$, d_k are the creation and annihilation operators of electrons and of holes, respectively, and k is the wave vector.

The scalar-potential Hamiltonian $H_{\mathcal{E}}$ describes the action of the applied uniform electric field $\mathcal{E}(t)$. In a semiconductor $H_{\mathcal{E}}$ splits into an accelerating part $H_\parallel$ and a polarizing part $H_\perp$ (Ref. 17)

$$H_{\mathcal{E}} = H_\parallel + H_\perp , \tag{3}$$

where the interband matrix elements Z_{cv} of $H_\parallel$ are zero. As a consequence $H_\parallel$ is diagonal with respect to the bands and thus describes intraband processes. It can be written as

$$H_\parallel = \sum_{k_1,k_2} Z_{cc}(k_1,k_2)\, c_{k_1}^\dagger c_{k_2} + \sum_{k_1,k_2} Z_{vv}(k_1,k_2)\, d_{k_1}^\dagger d_{k_2} , \tag{4}$$

where

$$Z_{ii}(k_1,k_2) = \frac{1}{V}\int d^3x\, \varphi_i^*(k_1,x) \times \left(-ie\mathcal{E}(t)\frac{\partial}{\partial k_2}\right) \varphi_i(k_2,x) , \tag{5}$$

($i = c$ or $i = v$). In the above expression $\varphi_i(k,x)$ are Bloch waves

$$\varphi_i(k,x) = \frac{1}{\sqrt{V}} e^{i\,k\cdot x} u_i(k,x)\,, \tag{6}$$

with periodic parts u_i and V is the volume.

The matrix elements $X_{ij}(k,k')$ of the polarizing part $H_\perp$ are zero for $k \neq k'$. By absorbing contributions of the form $X_{ii}(k,k)$ in H_0 [renormalization of the band energies $E_i(k)$], $H_\perp$ can be written as

$$H_\perp = \sum_k X_{vc}(k)\, c_k^\dagger d_{-k}^\dagger + \sum_k X_{vc}^*(k)\, d_{-k} c_k\,, \tag{7}$$

$$X_{vc}(k) = \frac{1}{V} \int d^3x\, u_c^*(k,x) \left(ie\mathcal{E}(t) \frac{\partial}{\partial k} \right) u_v(k,x)\,, \tag{8}$$

and consequently is nondiagonal with respect to the bands in contrast to $H_\parallel$ and thus describes interband processes.

The time evolution of the Bloch waves due to $H_\parallel$ is given by

$$\begin{aligned} U_t(H_\parallel)\varphi_i(k_0,x) &\equiv e^{-i\int_{t_0}^t H_\parallel d\tau/\hbar} \varphi_i(k_0,x) \\ &= \varphi_i(k_t,x)\,, \\ k_t &\equiv k_0 - \int_{t_0}^t \frac{e\mathcal{E}(\tau)}{\hbar} d\tau\,. \end{aligned} \tag{9}$$

$H_\parallel$ changes the crystal momentum of a Bloch carrier with time as $H_\mathcal{E}$ does for a free carrier in vacuum. In contrast to $H_\parallel$ the polarizing part of the electric field $H_\perp$ mixes states of different bands with same k (see above). In terms of transport this means that $H_\perp$ induces "vertical" Zener transitions from one band to the other (see Fig. 1).

The perturbation Hamiltonian H_1, in principle, represents a sum of all interaction mechanisms present in a semiconductor. Among them carrier-phonon and carrier-carrier interactions are the most important ones in pure materials. Carrier-carrier interaction, in turn, splits up, within the electron-hole picture, into several conceptually different contributions.[18] Here we will concentrate on the part that yields impact ionization and its inverse process, Auger recombination. The corresponding Hamiltonian is given by

$$\begin{aligned} H_1 = \sum_{k,k',q} \Big[& M_e(q) c_{k+q}^\dagger c_{k'-q}^\dagger d_{-k'}^\dagger c_k \\ & + M_e^*(q) c_k^\dagger d_{-k'} c_{k'-q} c_{k+q} \Big] \\ + \sum_{k,k',q} \Big[& M_h(q) d_{k+q}^\dagger d_{k'-q}^\dagger c_{-k'}^\dagger d_k \\ & + M_h^*(q) d_k^\dagger c_{-k'} d_{k'-q} d_{k+q} \Big]\,, \end{aligned} \tag{10}$$

where

$$M_e(q) = \frac{e^2}{\epsilon\epsilon_0 V} \frac{F_{cc} F_{vc}}{q^2+\lambda^2}\,, \quad M_h(q) = \frac{e^2}{\epsilon\epsilon_0 V} \frac{F_{vv} F_{cv}}{q^2+\lambda^2} \tag{11}$$

are the usual Debye-like screened Coulomb matrix elements. In these expressions λ is the inverse screening length, $F_{ij}(k,q)$ are the overlap (or Bloch) integrals, ϵ, ϵ_0 are the relative and absolute permittivity, and V is the crystal volume. H_1 describes impact-ionization processes and their inverse, Auger recombination initiated by electrons (index e) (see Fig. 2) and by holes (index h). The matrix elements for the electron and hole processes are different due to the different overlap integrals involved. Furthermore, since $F_{vc}(k,0) = 0$, we assume throughout the following $M_{e,h}(0) = 0$.

In the definition of our Hamiltonian we have suppressed the additional dependence on the spin variables.

B. The density-matrix approach

Time-independent solutions of the system $H_0 + H_\parallel$ form a discrete system of eigenfunctions, the so-called

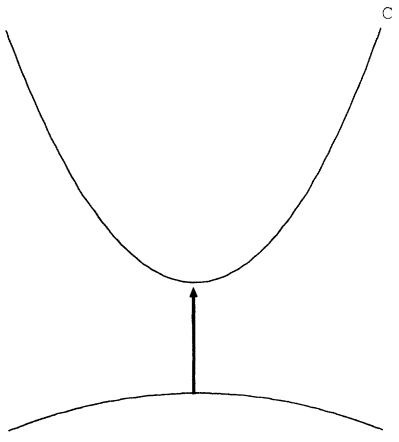

FIG. 1. Vertical interband process induced by the operator $H_\perp$. The conduction band (c) and the valence band (v) are schematically shown.

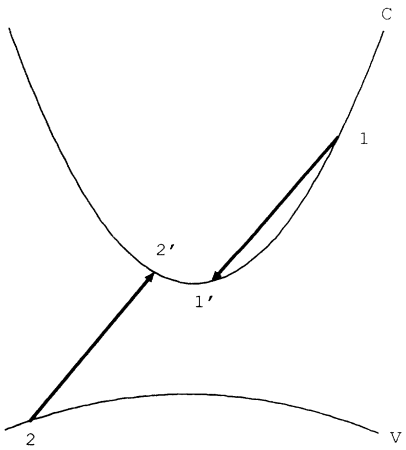

FIG. 2. Impact-ionization process. A conduction electron in state 1 collides with a valence electron in state 2, with the result that both electrons after the collision are in the conduction band in states 1′ and 2′, respectively.

Wannier-Stark ladder[19] with energy spacing $e\mathcal{E}d$ where d is the lattice constant. They are used in Ref. 11 to calculate the Zener transition rate. In semiconductor transport experiments a Wannier-Stark ladder in a band can only form if the total potential drop across the semiconductor exceeds the band width[20] that corresponds to the possibility for a Bloch oscillation. Furthermore, to perform at least one Bloch oscillation (to resolve the energy spacing $e\mathcal{E}d$) the carrier must not be scattered within the corresponding time interval. For electrons in the conduction band of a nondegenerate bulk semiconductor this requires an unreasonably high electric field. For this reason, and because we are explicitly interested in the time evolution of the system (1), we use a different (time-dependent) approach which we describe below.

1. The dynamics of the distribution function

The time evolution of the physical system described by H is reflected in the time evolution of the associated density matrix. The diagonal parts of the single-particle density matrices are given by the electron and hole distribution functions

$$f_e(k,t) \equiv \left\langle c_k^\dagger c_k \right\rangle \quad \text{and} \quad f_h(k,t) \equiv \left\langle d_k^\dagger d_k \right\rangle , \tag{12}$$

where $\langle\,\rangle$ denotes the ensemble average. Using time-dependent Bloch functions $\varphi_i(k_t,x)$ from Eq. (9) eliminates $H_\parallel$ from the equations of motion for $f_i(k_t,t)$ [see Eq. (A2) in Appendix A]. Since H_0 commutes with $c_{k_t}^\dagger c_{k_t}$, we obtain from (A2) two contributions for the total time derivative of f_e

$$\frac{d}{dt} f_e(k_t,t) = \frac{d}{dt} f_e(k_t,t)\Big|_{H_\perp} + \frac{d}{dt} f_e(k_t,t)\Big|_{H_1} . \tag{13}$$

The first term on the right-hand side (rhs) of (13) yields the interband generation rate

$$\frac{d}{dt}\, f_e(k_t,t)|_{H_\perp} = \frac{1}{i\hbar} X_{vc}(k_t)\, p^*(k_t,t) \;+\; \text{c.c.}\,, \tag{14}$$

where p is the interband polarization

$$p(k,t) \equiv \langle d_{-k} c_k \rangle , \qquad p^*(k,t) \equiv \left\langle c_k^\dagger d_{-k}^\dagger \right\rangle . \tag{15}$$

The second term on the right-hand side of Eq. (13) describes generation due to Coulomb interaction between carriers in different bands and is given by

$$\frac{d}{dt}\, f_e(k_t,t)|_{H_1} = \frac{1}{i\hbar} \sum_{k',q} \Big\{ M_e(q)\,[y_{e2} - y_{e1} + y_{e3}] + M_h(q) y_{e4} \Big\} \;+\; \text{c.c.}\,, \tag{16}$$

where

$$y_{e1} \equiv \left\langle c_{k+q}^\dagger c_{k'-q}^\dagger d_{-k'}^\dagger c_k \right\rangle ,$$

$$y_{e2} \equiv \left\langle c_k^\dagger c_{k'}^\dagger d_{-(k'+q)}^\dagger c_{k-q} \right\rangle , \tag{17}$$

$$y_{e3} \equiv \left\langle c_{k'}^\dagger c_k^\dagger d_{-(k+q)}^\dagger c_{k'-q} \right\rangle ,$$

$$y_{e4} \equiv \left\langle d_{-(k'-q)}^\dagger d_{-(k+q)}^\dagger c_k^\dagger d_{-k'} \right\rangle . \tag{18}$$

The y_{en} can be interpreted as the impact-ionization scattering amplitudes. For example, y_{e1} describes the process where, in the language of second quantization, an electron is destroyed in state k and created in $k+q$ thereby generating an electron-hole pair in $k'-q$ and $-k'$. This describes an impact-ionization event (see Fig. 2). The four contributions on the rhs of (16) reflect the four different impact-ionization processes that change the occupation of state k_t; they are the quantum mechanical analog of four corresponding transition rates in the semiclassical Boltzmann equation.[21] In (16) $e1$, $e2$, and $e3$ describe electron impact ionization, while $e4$ describes hole impact ionization.

We see that the equations for f_e (and f_h) couple to the polarization p, i.e., the interband elements of the one-particle density matrix, and to elements of the two-particle density matrix. The polarization p and the impact-ionization scattering amplitudes y_{en} must be obtained by solving their differential equations which in turn can be derived from Eq. (A2).

2. The dynamics of the polarization

The equation of motion for the polarization reads

$$\frac{d}{dt} p(k_t,t) = \frac{d}{dt}\, p(k_t,t)|_{H_0} + \frac{d}{dt}\, p(k_t,t)|_{H_\perp} + \frac{d}{dt}\, p(k_t,t)|_{H_1} , \tag{19}$$

and the three contributions are

$$\frac{d}{dt}\, p(k_t,t)|_{H_0} = \frac{1}{i}\Omega_p(k_t) p(k_t,t)\,,$$

$$\Omega_p(k) \equiv \frac{1}{\hbar}\left[E_c(k) + E_v(k)\right] , \tag{20}$$

$$\frac{d}{dt}\, p(k_t,t)|_{H_\perp} = \frac{1}{i\hbar} X_{vc}(k_t)\, \mathcal{F}_{eh}(k_t,-k_t,t)\,, \tag{21}$$

where

$$\begin{aligned}\mathcal{F}_{ij}(k,k',t) &= [1-f_i(k,t)][1-f_j(k',t)] \\ &\quad - f_i(k,t) f_j(k',t) \\ &= 1 - f_i(k,t) - f_j(k',t)\,, \quad i,j \in \{e,h\}\,,\end{aligned} \tag{22}$$

is the filling factor due to the Pauli principle. The last term on the rhs of Eq. (19) yields

$$\begin{aligned}\frac{d}{dt}\, p(k_t,t)|_{H_1} = &-\frac{1}{i\hbar}\sum_{k',q} \{M_e(q) y^{ee} - M_h(q) y^{hh} \\ &+ M_e(q) y_{p1}^e - M_h(q) y_{p1}^h\} \\ &-\frac{1}{i\hbar}\sum_{k',q} \{M_e(q) y_{p2}^e - M_h(q) y_{p2}^h \\ &+ M_e^*(q) y_{p3}^e - M_h^*(q) y_{p3}^h\} ,\end{aligned} \tag{23}$$

where

$$y^{ee} \equiv \left\langle c^\dagger_{k-q} c^\dagger_{k'+q} c_{k'} c_k \right\rangle , \; y^{hh} \equiv \left\langle d^\dagger_{-(k-q)} d^\dagger_{-(k'+q)} d_{-k'} d_{-k} \right\rangle , \; y^e_{p1} \equiv \left\langle c^\dagger_{k'-q} d_{-k} d^\dagger_{-k'} c_{k-q} \right\rangle ,$$
$$y^h_{p1} \equiv \left\langle d^\dagger_{-(k'-q)} c_k c^\dagger_{k'} d_{-(k-q)} \right\rangle , \; y^e_{p2} \equiv \left\langle d_{-k} c^\dagger_{k'+q} d^\dagger_{-(k+q)} c_{k'} \right\rangle , \; y^h_{p2} \equiv \left\langle c_k d^\dagger_{-(k'+q)} c^\dagger_{k+q} d_{-k'} \right\rangle ,$$
$$y^e_{p3} \equiv \left\langle d_{-k} d_{-(k'+q)} c_{k+q} c_{k'} \right\rangle , \; y^h_{p3} \equiv \left\langle d_{-k'} d_{-(k+q)} c_{k'+q} c_k \right\rangle .$$

The polarization thus couples to the distribution functions f_e, f_h, and to further elements of the two-particle density matrix associated with electron-electron, hole-hole, and electron-hole scattering.

3. *The dynamics of the impact-ionization scattering amplitude*

It is here sufficient to consider only y_{e1} because the equations of motion for the other impact-ionization scattering amplitudes can be obtained from permutations. The time derivative of y_{e1} is determined again with the aid of Eq. (A2)

$$\frac{d}{dt} y_{e1} = \frac{d}{dt} y_{e1}|_{H_0} + \frac{d}{dt} y_{e1}|_{H_\perp} + \frac{d}{dt} y_{e1}|_{H_1} . \tag{24}$$

In the last equation the first term on the rhs gives the energy difference between the initial and the final two-particle state multiplied by y_{e1}

$$\frac{d}{dt} y_{e1}|_{H_0} = i\Omega_{e1}(t)\, y_{e1} , \tag{25}$$

where

$$\Omega_{e1}(t) = \frac{1}{\hbar}[E_c(k_t+q) + E_c(k'_t - q) + E_v(k'_t) - E_c(k_t)] . \tag{26}$$

The second term obviously leads to the same type of density matrices as appear in Eq. (23)

$$\begin{aligned}\frac{d}{dt} y_{e1}|_{H_\perp} = {} & \frac{i}{\hbar} X^*_{vc}(k_t+q) \left\langle d_{-(k_t+q)} c^\dagger_{k'_t-q} d^\dagger_{-k'_t} c_{k_t} \right\rangle \\ & - \frac{i}{\hbar} X^*_{vc}(k'_t) \left\langle c^\dagger_{k_t+q} c^\dagger_{k'_t-q} c_{k'_t} c_{k_t} \right\rangle \\ & + \frac{i}{\hbar} X^*_{vc}(k'_t - q) \left\langle c^\dagger_{k_t+q} d_{-(k'_t-q)} d^\dagger_{-k'_t} c_{k_t} \right\rangle \\ & - \frac{i}{\hbar} X_{vc}(k_t) \left\langle c^\dagger_{k_t+q} c^\dagger_{k'_t-q} d^\dagger_{-k'_t} d^\dagger_{-k_t} \right\rangle . \end{aligned} \tag{27}$$

The third term leads to three-particle density matrices. For example, the commutator of y_{e1} with the electron Auger recombination term yields

$$\left\langle \left[\sum_{k'',k''',q'} M^*_e(q) c^\dagger_{k''} d_{-k'''} c_{k'''-q'} c_{k''+q'} \, , \, c^\dagger_{k+q} c^\dagger_{k'-q} d^\dagger_{-k'} c_k \right] \right\rangle$$

$$\begin{aligned} = {} & \sum_{k'',q'} M^*_e(q') \left\langle \left\{ c^\dagger_{k+q-q'} d_{-(k''+q')} c_{k''} c^\dagger_{k'-q} - c^\dagger_{k'-q-q'} d_{-(k''+q')} c_{k''} \, c^\dagger_{k+q} \right\} d^\dagger_{-k'} \, c_k \right\rangle \\ & + \sum_{k'',q'} M^*_e(q') \left\langle \left\{ c^\dagger_{k''-q'} d_{-(k+q+q')} c^\dagger_{k'-q} - c^\dagger_{k''-q'} d_{-(k'-q+q')} c^\dagger_{k+q} \right\} d^\dagger_{-k'} c_k c_{k''} \right\rangle \\ & + \sum_{k'',q'} M^*_{q'}(q) \left\langle c^\dagger_{k+q} c^\dagger_{k'-q} \left\{ c^\dagger_{k''-q'} \, c_k c_{k'-q'} c_{k''} - d^\dagger_{-k'} d_{-(k''+q')} c_{k''} c_{k+q'} \right\} \right\rangle . \end{aligned} \tag{28}$$

The remaining permutations give similar results.

This scheme leads to a system of an infinite number of coupled differential equations. In order to close it, this hierarchy must be truncated within some approximation scheme which we will present in the next section.

III. SYSTEM OF KINETIC EQUATIONS

In this section we want to close the previously obtained hierarchy of differential equations for our principal variables: the distribution functions f_e and f_h [Eq. (13)], the polarization p [Eq. (19)], and the impact-ionization scattering amplitudes y_{e1}, y_{e2}, y_{e3}, and y_{e4} [Eq. (24)]. All other n-particle density matrices will be split into sums of all possible products of those principal variables. This amounts to a mean field approximation. For example, the first term on the rhs of Eq. (23) is approximated by a sum of two products of two distribution functions

$$\left\langle c^\dagger_{k-q} c^\dagger_{k'+q} c_{k'} c_k \right\rangle \approx \delta_{q,0} \left\langle c^\dagger_k c_k \right\rangle \left\langle c^\dagger_{k'} c_{k'} \right\rangle - \delta_{k,k'+q} \left\langle c^\dagger_k c_k \right\rangle \left\langle c^\dagger_{k-q} c_{k-q} \right\rangle . \tag{29}$$

In this case the above decoupling coincides with the usual

Hartree-Fock approximation where the first and the second term correspond to the direct Coulomb and the exchange interaction, respectively. Other terms of the rhs of Eq. (23) decouple into products of a distribution function and a polarization. In the same manner we treat the three-particle density matrices with six mode operators. For example, the third term on the rhs of Eq. (28) decouples into the following products:

$$\begin{aligned}\left\langle c^\dagger_{k''+q'} d_{-(k+q-q')} c^\dagger_{k'-q} d^\dagger_{-k'}\, c_k c_{k''}\right\rangle \approx\ & [1-f_h(-k')] f_e(k'-q) f_e(k) \delta_{k'',k'-q}\delta_{q',k+q-k'} \\ & -[1-f_h(-k')] f_e(k'') f_e(k) \delta_{q',0}\delta_{q',k+q-k'} \\ & -p(k) p^*(k') f_e(k'-q)\delta_{q',q}\delta_{k'',k'-q} - y_{e1}(k,k',q,t) p(k+q-q')\delta_{k'',k+q-q'}\,. \end{aligned} \tag{30}$$

All terms containing $\delta_{q,0}$ or $\delta_{q',0}$ can be neglected because $M_e(0)$ and $M_h(0)$ are zero (due to vanishing overlap integrals for $q \to 0$).

The situation of the y_{en} terms is more complicated. They already contain contributions that are products of distribution functions and of polarizations. This is seen by applying the Hartree-Fock approximation to y_{e1} as a first-order approximation

$$\begin{aligned} y_{e1} &\approx \delta_{q,0}\left\langle c^\dagger_k c_k\right\rangle \left\langle c^\dagger_{k'} d^\dagger_{-k'}\right\rangle \\ &\quad -\delta_{k+q,k'}\left\langle c^\dagger_k c_k\right\rangle \left\langle c^\dagger_{k+q} d^\dagger_{-(k+q)}\right\rangle \\ &= \delta_{q,0}\, f_e(k,t)\, p^*(k',t) - \delta_{k+q,k'}\, f_e(k,t)\, p^*(k+q,t)\,, \end{aligned} \tag{31}$$

where the first term on the right-hand side due to $q=0$ can be neglected.

In a systematic expansion of the hierarchy of correlations we shall now consider the deviation from the Hartree-Fock factorized form as a second-order contribution

$$s_{e1}(t) \equiv y_{e1}(t) + \delta_{k+q,k'}\, f_e(k,t)\, p^*(k+q,t)\,. \tag{32}$$

This is a measure for the two-particle correlation in the impact-ionization process, and will be denoted as impact-ionization density-correlation function. If we limit the influence of H_1 to its first-order coherent contribution we must neglect s_{e1}. Otherwise we must consider an additional differential equation for s_{e1}. According to Eq. (32), we have to evaluate

$$\begin{aligned}\frac{d}{dt} s_{e1} = \frac{d}{dt} y_{e1} + \delta_{k+q,k'}\Big[&\left(\frac{d}{dt} f_e(k,t)\right) p^*(k+q,t) \\ &+ f_e(k,t)\left(\frac{d}{dt} p^*(k+q,t)\right)\Big]. \end{aligned} \tag{33}$$

Analogously, we define

$$s_{e2}(t) \equiv y_{e2}(t) + \delta_{k,k'+q}\, f_e(k-q,t)\, p^*(k,t)\,, \tag{34}$$

$$s_{e3}(t) \equiv y_{e3}(t) + \delta_{k+q,k'}\, f_e(k,t)\, p^*(k+q,t)\,, \tag{35}$$

$$s_{e4}(t) \equiv y_{e4}(t) - \delta_{k+q,k'}\, f_h(k+q,t)\, p^*(k,t)\,. \tag{36}$$

In a consistent scheme, besides $f_{e,h}$ and p, the pure two-particle correlations s_{en}, rather than y_{en}, must be used as additional dynamic variables.

A. The semiconductor Bloch equations in the accelerated frame

We obtain for Eq. (16)

$$\begin{aligned}\frac{d}{dt} f_e(k_t,t)|_{H_1} = &\frac{1}{i\hbar}\Delta_p(k_t) p^*(k_t,t) \\ &+\frac{1}{i\hbar}\sum_{k',q}\{M_e(q)\,[s_{e2}-s_{e1}+s_{e3}] \\ &+M_h(q) s_{e4}\} + \text{c.c.}\,, \end{aligned} \tag{37}$$

and, using the Hartree-Fock approximation (29), for Eq. (23)

$$\begin{aligned}\frac{d}{dt} p^*(k_t,t)|_{H_1} \approx &\frac{i}{\hbar}\Sigma_p(k_t) p^*(k_t,t) \\ &+\frac{i}{\hbar}\Delta^*_p(k_t)\,\mathcal{F}_{eh}(k_t,-k_t,t)\,, \end{aligned} \tag{38}$$

where we have introduced the self-energy Σ_p

$$\begin{aligned}\Sigma_p(k) \equiv -\sum_{q'}\{&[M_e(q')-M_h(q')]\, p^*(k+q') \\ &+[M_e(q')-M_h(q')]^*\, p(k+q')\} \end{aligned} \tag{39}$$

and the internal field Δ_p

$$\begin{aligned}\Delta_p(k) \equiv -\sum_{q'}\{&M_e(q')\, f_e(k-q') \\ &-M_h(q')\, f_h[-(k-q')]\}\,. \end{aligned} \tag{40}$$

Equation (37) is exact, while in (38) we have neglected the two-particle correlations associated with carrier-carrier scattering processes. This is justified for not too large carrier densities (weak carrier-carrier scattering). The self-energy Σ_p is real and expresses the first-order coherent contribution of impact ionization and Auger recombination to the polarization. It can also be interpreted as a renormalization of the electron and hole band energies $E_c(k)$ and $E_h(k)$ in (20) due to impact ionization and Auger recombination induced polarization according to

$$E_c(k) - \sum_{q'} \{M_e(q')\, p^*(k+q') + M_e^*(q')\, p(k+q')\}\,, \tag{41}$$

$$E_v(k) + \sum_{q} \{M_h(q)\, p^*(k+q) + M_h^*(q)\, p(k+q)\}\,. \tag{42}$$

$E_c(k)$ and $E_v(k)$ are shifted in different "directions," such that the effect on the band gap may partially cancel. The internal field Δ_p can be interpreted as a Coulomb enhancement of the interband matrix element X_{vc} thus renormalizing the external field $\mathcal{E}$.

If we neglect in Eq. (37) the impact-ionization density-correlation contribution then we obtain a closed system of equations for the distribution functions f_e and f_h and for the polarization p. Without the explicit time dependence of the wave vectors due to $H_{\|}$ this system would coincide with the semiconductor Bloch equations.[14,22] They describe a set of two-level systems modified by the presence of additional scattering processes (contained in H_1)[23]

$$\frac{d}{dt} f_{e/h}(k_t,t)\big|_{\text{Bloch}} = \frac{1}{i\hbar}\left[\{X_{vc}(k_t) + \Delta_p(k_t)\}\, p^*(k_t,t) - \{X_{vc}(k_t) + \Delta_p(k_t)\}^*\, p(k_t,t)\right], \tag{43}$$

$$\frac{d}{dt} p^*(k_t,t)\big|_{\text{Bloch}} = i\,\{\Omega_p(k_t) + \Sigma_p(k_t)/\hbar\}\, p^*(k_t,t) + \frac{i}{\hbar}\left[\{X_{vc}(k_t) + \Delta_p(k_t)\}^* \times \mathcal{F}_{eh}(k_t,-k_t,t)\right]. \tag{44}$$

It is seen that the importance of impact ionization for the total self-energy and internal field depends on the difference of the overlap integrals within different bands. The internal field contribution, on the other hand, depends also on the difference of the electron and hole distribution functions.

B. A quantum kinetic equation for impact ionization

We will now extend the above system of semiconductor Bloch equations by including in our set of kinetic variables the impact-ionization density-correlation functions s_{en}. This is obtained by taking into account the various s_{en} terms in the equations for the distribution functions and by deriving additional equations of motion for the s_{en} terms themselves. According to Eq. (33), the derivatives of f_e and p^* are needed. In order to be consistent with our approximation scheme, here these time derivatives are given by the Bloch equations Eq. (43) and Eq. (44). Therefore, we are left with the determination of the last commutator in Eq. (24), which after mean field approximation reads

$$\left.\frac{d}{dt} y_{e1}\right|_{H_1} = \frac{i}{\hbar}\bar{M}_e^*(q)\mathcal{F}_{e1}(t) + \frac{i}{\hbar} y_{e1}\,\Sigma_{e1}(k_t,k_t',q) + \delta_{k_t+q,k_t'}\frac{i}{\hbar}\tilde{\mathcal{W}}_{e1}(k_t,k_t+q) + \frac{i}{\hbar}\mathcal{W}_{e1}(k_t,k_t',q)\,, \tag{45}$$

where

$$\bar{M}_i(q) \equiv M_i(q) - \tfrac{1}{2} M_i(k'-q-k)\,, \quad i\epsilon\{e,h\} \tag{46}$$

and

$$\mathcal{F}_{e1}(t) = f_e(k,t)\,[1-f_e(k+q,t)]\,[1-f_h(-k',t)] \times [1-f_e(k'-q,t)] - [1-f_e(k,t)] \times f_e(k+q,t)\, f_h(-k',t)\, f_e(k'-q,t) \tag{47}$$

assures that in the impact ionization (first part) and the Auger recombination (second part) transitions the Pauli principle is always fulfilled. The real self-energy

$$\Sigma_{e1}(k,k',q) \equiv -\sum_{q'}\{M_e^*(q')\,[p(k+q+q') + p(k'-q+q') - p(k+q')] - M_h^*(q')p(k'+q') + \text{c.c.}\} \tag{48}$$

corrects the band energy of the four states here in the same way as we have already seen for the polarization. The next term

$$\tilde{\mathcal{W}}_{e1}(k,k+q) \equiv p^*(k+q)\,[p^*(k)\,\Delta_p(k) - \Delta_p^*(k)\,p(k)] - \Delta_p^*(k+q) f_e(k)\,\mathcal{F}_{eh}(k+q,k+q) \tag{49}$$

describes virtual impact-ionization transitions in which energy cannot be conserved. The last term, finally, describes how polarization due to the Coulomb interaction can result in real impact ionization or Auger recombination according to the occupation of the electron or hole states

$$\mathcal{W}_{e1}(k,k',q) = \bar{M}_e^*(q)\,p(k)p^*(k')\mathcal{F}_{ee}(k+q,k'-q) - \bar{M}_h^*(q)\,p(k)p^*(k+q)\mathcal{F}_{eh}(k'-q,-k') - \bar{M}_h^*(q)\,p(k)p^*(k'-q)\mathcal{F}_{eh}(k+q,-k') + \bar{M}_h(q)\,p^*(k+q)p^*(k'-q)\mathcal{F}_{eh}^2(k,-k') - \bar{M}_e(q)\,p^*(k')p^*(k'-q)\mathcal{F}_{ee}^2(k,k+q) - \bar{M}_e(q)\,p^*(k')p^*(k+q)\mathcal{F}_{ee}^2(k,k'-q)\,. \tag{50}$$

Here we have additionally introduced

$$\mathcal{F}^2_{ij}(k,k') \equiv f_i(k)[1-f_j(k')] - f_j(k')[1-f_i(k)]\,,$$

$$i,j\epsilon\{e,h\}\,. \quad (51)$$

Setting up the equations for the s_{en} we see that the $\tilde{\mathcal{W}}_{en}$ terms cancel completely due to the last term of Eq. (33) and due to the mean field approximation for Eq. (27). Since $\Sigma_p(k+q)$ and $\Sigma_{e1}(k,k+q,q)$ coincide we obtain for s_{e1}

$$\frac{d}{dt}s_{e1} = i\left\{\Omega_{e1}(t) + \Sigma_{e1}(k_t,k'_t,q)/\hbar\right\} s_{e1} + \frac{i}{\hbar}\bar{M}_e(q)\mathcal{F}_{e1}(t) + \frac{i}{\hbar}\mathcal{W}_{e1}(k_t,k'_t,q)\,. \quad (52)$$

The $\mathcal{W}$ terms, in general, oscillate since they contain products of the polarization, and their integral contribution to the s_{en} terms should be small compared to the $\bar{M}_e(q)\,\mathcal{F}_{en}(t)$ terms for those (k,k',q) which approximately conserve energy. Especially for the first term on the rhs of Eq. (50) this assumption may not always be justified.

Putting all together, our closed system for the distribution functions, the polarization, and the impact-ionization density-correlation functions becomes

$$\frac{d}{dt}f_e(k_t,t) = \frac{1}{i\hbar}\left[\{X_{vc}(k_t)+\Delta_p(k_t)\}\,p^*(k_t,t) - \text{c.c.}\right] + \frac{1}{i\hbar}\left[\sum_{k',q}\left\{M_e(q)\,(s_{e2}-s_{e1}+s_{e3}) + M_h(q)s_{e4}\right\} - \text{c.c.}\right], \quad (53)$$

an analogous equation for f_h,

$$\frac{d}{dt}p^*(k_t,t) = i\left\{\Omega_p(k_t)+\Sigma_p(k_t)/\hbar\right\}p^*(k_t,t) + \frac{i}{\hbar}\{X_{vc}(k_t)+\Delta_p(k_t)\}^*\,\mathcal{F}_{eh}(k_t,-k_t,t)\,, \quad (54)$$

and four equations ($j=1,2,3,4$) of the form

$$\frac{d}{dt}s_{ej}(t) = i\left\{\Omega_{ej}(t)+\Sigma_{ej}(k_t,k'_t,q)/\hbar\right\}s_{ej} + \frac{i}{\hbar}\left[\bar{M}_{e_j}(q)\mathcal{F}_{ej}(t)+\mathcal{W}_{ej}(k_t,k'_t,q)\right]\,. \quad (55)$$

In the last term we have additionally used $e_j = e(j=1,2,3)$ and $e_4 = h$. The equations for the distribution functions are coupled for the same k through $H_\perp$ and through the internal field due to the first-order coherent contribution of impact ionization and Auger recombination, and for different k' through the second-order contribution of impact ionization and Auger recombination. The first and the second square brackets in (53) describe generation rates due to polarization and impact ionization, respectively.

The equations for the polarization and the impact-ionization density-correlation functions both are of the type

$$\frac{d}{dt}a(t) = i\Omega(t)\,a(t) + \Gamma(t)\,, \quad (56)$$

which can formally be integrated yielding

$$a(t) = a(t_0)\exp\left\{i\int_{t_0}^{t}\Omega(\tau)d\tau\right\} + \int_{t_0}^{t}\exp\left\{i\int_{t'}^{t}\Omega(\tau)d\tau\right\}\Gamma(t')dt'\,. \quad (57)$$

If we neglect self-energy corrections and $\mathcal{W}_{en}$, the equations for the polarization and for the impact-ionization density-correlation functions are not directly coupled. So with the above formal integration $p(k,t)$ and $s_{en}(t)$ can be eliminated resulting in equations only for the distribution functions. As we will show in the next two sections, for the polarization this will lead to the well-known Zener effect, and for the impact-ionization density-correlation functions to field-assisted impact-ionization scattering.

IV. POLARIZATION-INDUCED CARRIER GENERATION

In the last section, we have derived a differential equation for f_e, with two generation terms, generation by polarization and by impact ionization. In this section, we will deal with the first one. We show that both the Zener effect and the Franz-Keldysh effect can be obtained straightforwardly from the semiconductor Bloch equations in the accelerated frame.

A. The Zener effect

By neglecting the self-energy $\Sigma_p(k)$, the differential equation (44) for p^* can be integrated according to Eq. (57). By defining

$$\bar{X}_{vc}(k) \equiv X_{vc}(k) + \Delta_p(k), \quad (58)$$

the following equation for the contribution of the polarization to the rate of change for $f_e(k)$ is obtained,

$$\left.\frac{d}{dt}f_e(k_t,t)\right|_Z = \frac{2}{\hbar^2}\,\text{Re}\left[\bar{X}_{vc}(k_t)\int_{t_0}^{t}dt' \times\exp\left\{i\int_{t'}^{t}d\tau\;\Omega_p(k_\tau)\right\}\bar{X}^*_{vc}(k_{t'}) \times\mathcal{F}_{ek}(k_{t'},-k_{t'},t')\right], \quad (59)$$

assuming that at $t=t_0$ no polarization exists, i.e., $p^*(k,t_0)=0$. The above equation can further be elaborated analytically assuming that the phase space filling factor $\mathcal{F}_{eh}(k,-k,t)$ is close to unity (nondegenerate limit) which is often a good approximation in the high-field region of a semiconductor device. Assuming a direct

semiconductor, we will see that the only relevant nonassisted Zener processes take place in the vicinity of the band edges. Therefore, one can approximate $\bar{X}_{vc}(k)$ by $\bar{X}_{vc}(0)$. The Zener transition rate, i.e., the total number of electrons entering the conduction band per unit time, is then obtained from Eq. (59) by summing over all k_t (expressed by dimensionless components $\kappa_\parallel$ and $\kappa_\perp$ parallel and perpendicular to the field $\mathcal{E}$) and performing the limit $t_0 \to -\infty$,

$$\frac{dn}{dt} = C_Z \int d\kappa_\perp^2 \int_{-\infty}^{\infty} d\kappa_\parallel \int_{-(t-t_0)}^{t-t_0} d\tau \times \cos\left(\tau \frac{\omega_g + \omega_\perp}{\omega_F} + \frac{1}{3}\tau^3 + \kappa_\parallel \frac{\omega_g + \omega_\perp}{\omega_F} + \frac{1}{3}\kappa_\parallel^3\right) . \tag{60}$$

Here we have used the following abbreviations:

$$C_Z = 2\pi \frac{|\bar{X}_{vc}(0)|^2}{\hbar^2} \left(\frac{m^*}{2\pi^2\hbar}\right)^{3/2}, \quad m^* = \frac{m_c m_v}{m_c + m_v}, \tag{61}$$

$$\omega_g = E_g/\hbar, \quad \omega_\perp = \frac{\hbar k_\perp^2}{2m^*}, \quad \omega_F = \left(\frac{e^2\mathcal{E}^2}{2m^*\hbar}\right)^{1/3}, \tag{62}$$

where ω_F is called the electro-optical frequency. Expression Eq. (60) justifies the approximation $\bar{X}_{vc}(k_t) \approx \bar{X}_{vc}(0)$ since due to the rapidly oscillating integrand higher energy states give only a very small contribution. Due to the complete symmetry between the (dimensionless) time τ and $\kappa_\parallel$ in the argument of the cosine, the initial time t_0 becomes less and less important and we may take the limit $t_0 \to -\infty$. Then, in the Markov limit, the well-known result for the Zener tunneling rate in direct semiconductors[4] is obtained,

$$\frac{dn}{dt} = 2\frac{|\bar{X}_{vc}|^2}{\hbar^2} \left(\frac{m^*}{2\pi^2\hbar}\right)^{3/2} \sqrt{\pi\omega_F}\pi \left[\mathrm{Ai}'^2\left(\frac{\omega_g}{\omega_F}\right) - \frac{\omega_g}{\omega_F}\mathrm{Ai}^2\left(\frac{\omega_g}{\omega_F}\right)\right] , \tag{63}$$

where $\mathrm{Ai}(x)$ denotes the Airy function. Neglecting $\Delta_p(k)$ and using the following approximation for the interband matrix element X_{vc} (Ref. 24):

$$|X_{vc}|^2/\hbar^2 = \frac{e^2\mathcal{E}^2}{4m^* E_g}, \tag{64}$$

the Zener tunneling rate according to Eq. (63) is shown in Fig. 3 as a function of the electric field $\mathcal{E}$. For the calculation we used $m_c = 0.067\,m_0$, $m_v = 0.45\,m_0$, and $E_g = 1.422\,\mathrm{eV}$ which are typical values for GaAs at room temperature.

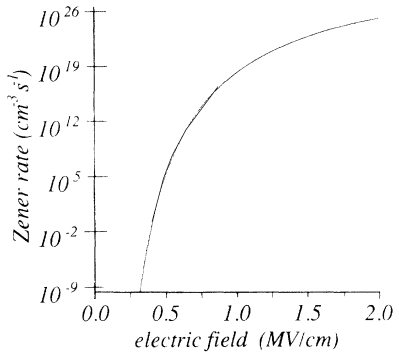

FIG. 3. Zener generation rate dn/dt as a function of the electric field $\mathcal{E}$ calculated for GaAs at $T = 300\,\mathrm{K}$.

B. The Franz-Keldysh effect

Let us now suppose that the electric field $\mathcal{E}$ is the sum of a static field $\mathcal{E}$ (due to an applied voltage) and an alternating electric field $\mathcal{E}_L$ as is present in laser light which, on a semiclassical level, can be described by[14]

$$H_L = \sum_k M_L(k)\mathcal{E}_L^{(+)} c_k^\dagger d_{-k}^\dagger + \sum_k M_L^*(k)\mathcal{E}_L^{(-)} d_{-k} c_k , \tag{65}$$

where the interband matrix element $X_{vc}(k)$ is split into the pure dipole matrix element $M_L(k)$ and the alternating electric field written as

$$\mathcal{E}_L^{(+)} = \mathcal{E}_0\, e^{-i\omega_L t}, \quad \mathcal{E}_L^{(-)} = \mathcal{E}^{(+)*} . \tag{66}$$

In the case where the electric field strength of the laser is much weaker than the electric field strength due to the applied external voltage, which in modern devices can easily be in the range of 10^5–10^6 V/cm, then the contribution of the laser to $H_\parallel$ is negligible. In $H_\perp$, on the other hand, the influence of the laser dominates because it can transfer energy to the electronic system. The Franz-Keldysh effect[25,26] occurs under these conditions and describes the creation of an electron-hole pair by a photon of frequency ω_L assisted by a strong static externally applied voltage. The calculation is the same as for the Zener effect except that in Eqs. (60) and (63) in addition to the replacement of the matrix element X_{vc} by $M_L\mathcal{E}_0$ one has to substitute ω_g with $\omega_g - \omega_L$. One obtains

$$\frac{dn}{dt} = \frac{1}{2}\Omega_R^2 \left(\frac{m^*}{2\pi^2\hbar}\right)^{3/2} \sqrt{\pi\omega_F}\pi \left[\mathrm{Ai}'^2(x) - x\mathrm{Ai}^2(x)\right] ,$$

$$x = \frac{\omega_g - \omega_L}{\omega_F} . \tag{67}$$

Here the amplitude $\mathcal{E}_0$ of the laser is given in terms of a Rabi frequency $\Omega_R = |2M_L(0)\mathcal{E}_0|/\hbar$. The electric field $\mathcal{E}$ from the externally applied constant voltage enters only through ω_F. For an electric field $\mathcal{E} = 10^6$ V/cm and a Rabi frequency of $\Omega_R = 5 \times 10^{12}\ \mathrm{s}^{-1}$ the generation rate due to a laser is shown in Fig. 4 as a function of the photon energy $\hbar\omega_L$. As is seen in Fig. 4 the threshold introduced by the band gap is softened by the Franz-Keldysh effect, i.e., even photons with energy below the gap are able to create an electron-hole pair. The extra energy is provided by the intracollisional field effect, i.e., the intra-

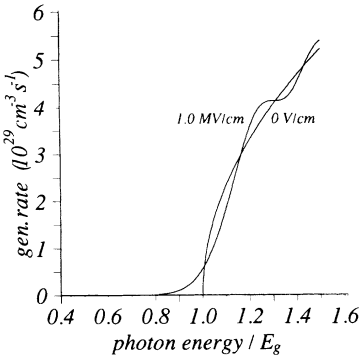

FIG. 4. Optical generation rate dn/dt due to a laser as a function of the photon energy (normalized to the band gap) with and without an external static field $\mathcal{E}$ (calculated for GaAs at $T = 300$ K).

band acceleration of carriers by the field due to $H_{\parallel}$. The range of the softening is of the order of $\hbar\omega_F$.[25] The generation rate given by (67) is proportional to the absorption coefficient,[15] i.e., the quantity that can be measured in experiments.

V. IMPACT-IONIZATION-INDUCED CARRIER GENERATION

In the previous section, in the derivation of the Franz-Keldysh effect we replaced $H_{\perp}$ with H_L. This results in the appearance of the frequency ω_L of the oscillating light field in the argument of the exponential function. Now we will show that in an impact-ionization process in the presence of an external electric field the impact-ionizing electron with energy $E_c(k)$ plays the role of the photon in the Franz-Keldysh effect such that the mathematical description remains almost unchanged. Here the energy (or part of it) of the impact-ionizing electron is used to create an electron-hole pair and this process is assisted by the presence of an electric field as in the case of the Franz-Keldysh effect.

A. The impact-ionization generation rate

In analogy with the polarization, Eq. (55) can be integrated according to (57), and the resulting expressions for the s_{en} can be inserted into Eq. (53). For simplicity we neglect in the following the $\mathcal{W}_{en}$ terms, and the self-energies Σ_{en}. The result of the integration is

$$\begin{aligned}\frac{d}{dt} f_e(k_t,t)|_{H_1} = &\frac{2\pi}{\hbar^2}\sum_{k',q}\int_{t_0}^{t} dt' \frac{1}{\pi}\cos\left\{\int_{t'}^{t} d\tau \Omega_{e2}(\tau)\right\} \mathcal{M}_e(k_{t'},k'_{t'},q)\, \mathcal{F}_{e2}(t') \\ &+\frac{2\pi}{\hbar^2}\sum_{k',q}\int_{t_0}^{t} dt' \frac{1}{\pi}\cos\left\{\int_{t'}^{t} d\tau \Omega_{e3}(\tau)\right\} \mathcal{M}_e(k_{t'},k'_{t'},q)\, \mathcal{F}_{e3}(t') \\ &-\frac{2\pi}{\hbar^2}\sum_{k',q}\int_{t_0}^{t} dt' \frac{1}{\pi}\cos\left\{\int_{t'}^{t} d\tau \Omega_{e1}(\tau)\right\} \mathcal{M}_e(k_{t'},k'_{t'},q)\, \mathcal{F}_{e1}(t') \\ &+\frac{2\pi}{\hbar^2}\sum_{k',q}\int_{t_0}^{t} dt' \frac{1}{\pi}\cos\left\{\int_{t'}^{t} d\tau \Omega_{e4}(\tau)\right\} \mathcal{M}_h(k_{t'},k'_{t'},q)\, \mathcal{F}_{e4}(t') \,. \end{aligned} \tag{68}$$

We have used the fact that, in a sum over k' and q, $M_i(q)\,\bar{M}_i^*(q)$ can be replaced by

$$\mathcal{M}_i(k,k',q) \equiv \frac{1}{4}\left(|M_i(q)|^2 + |M_i(q) - M_i(k'-q-k)|^2 + |M_i(k'-q-k)|^2\right), \; i\epsilon\{e,h\}\,. \tag{69}$$

The first term in Eq. (68) describes in-scattering of an electron from the conduction band into the state labeled by k and its inverse. The second describes in-scattering of an electron from the valence band into state k and its inverse. The third term describes out-scattering of an electron out of state k and its inverse. The fourth term finally describes in-scattering of an electron from the valence band due to hole impact ionization. In the above equation the rate of change of the electron distribution function at time t depends also on the distribution functions at earlier times, i.e., the dynamics is non-Markovian. Equation (68) supplemented by a similar equation for the distribution function of holes f_h represents a complicated but closed system of differential equations for the determination of the distribution functions.

In order to discuss some important differences with respect to the semiclassical approach and to emphasize the similarities with the Franz-Keldysh effect, we assume the case of a semiconductor device under conditions where in the high-field region the electron density is nondegenerate, and the hole density is negligible. Neglecting thus all terms containing M_h or products of distribution functions $f_e(k_1)f_e(k_2)$, and approximating terms of the type $(1-f)$ by unity one obtains the total impact-ionization rate dn/dt due to electron impact ionization only, by summing over k. Using the symmetry with respect to the summation variables, we find

$$\frac{dn(t)}{dt} = \sum_{k_t}\frac{2\pi}{\hbar^2}\int_{t_0}^{t} dt' f_e(k_{t'},t')\sum_{k',q}\frac{1}{\pi} \times \cos\left\{\int_{t'}^{t} d\tau \Omega_1(\tau)\right\} |M_e(q)|^2 \,, \tag{70}$$

where we have approximated $\mathcal{M}_e(k,k',q)$ by $|M_e(q)|$.[2,27] The last equation was analyzed in the ultrashort time regime in Refs. 28–30 assuming constant overlap integrals, and parabolic spherical valence and conduction bands. It was shown there that due to energy-time uncertainty and due to the applied strong electric field impact-ionization transitions take place even below the "semiclassical impact-ionization threshold" determined by energy and momentum conservation according to Fermi's golden rule.

B. Field-assisted impact ionization

In the following for simplicity we again assume a direct spherical parabolic semiconductor. The more complicated case of silicon is treated in Appendix B.

With these assumptions five of the six integrations over k' and q in Eq. (70) can be carried out analytically, and one obtains

$$\frac{dn(t)}{dt} = \int_{t_0}^{t} dt' \sum_{k_t} f_e(k_{t'},t') \int_0^{\omega_{\max}} d\omega \times S(\omega_f(k_{t_+}),\omega_f(k_{t_+})-\omega) \times \frac{1}{\pi}\cos\left(\frac{1}{3}(\omega_F^{ii}t_-)^3 + \frac{\bar{\omega}}{\omega_F^{ii}}(\omega_F^{ii}t_-)\right) \quad (71)$$

for the number of carriers that enter the conduction band per unit time and unit volume due to field-assisted impact-ionization. In the above expression

$$t_- \equiv t - t', \qquad t_+ \equiv (t+t')/2 \quad (72)$$

are the relative and absolute scattering times,

$$S(\omega_f,\omega) = \frac{1}{\tau}\left[\frac{1}{2}\left(\sqrt{\frac{\omega_f}{\omega_g^{\lambda}(\omega_f,\omega)}} + \sqrt{\frac{\omega_g^{\lambda}(\omega_f,\omega)}{\omega_f}}\right) - 1\right] \quad (73)$$

expresses the impact-ionization scattering rate with threshold energy $\mu^2\hbar\omega$ and impact-ionization mean free flight time τ defined by

$$\frac{1}{\tau} \equiv \frac{1}{\pi^2}\sqrt{\mu}(1+\alpha)^{-3/2}\left(\frac{e^2|F_{vc}F_{cc}|\sqrt{m_c}}{\epsilon\epsilon_0\hbar^{3/2}}\right)^2 . \quad (74)$$

The information about the particular band structure is contained in

$$\omega_f(k) = \frac{1}{\mu^2}\frac{\hbar k^2}{2m_c},$$

$$\omega_g^{\lambda}(\omega_f,\omega) = \frac{1}{2}\left(\sqrt{(\omega_\lambda-\omega)^2+4\omega_f\omega_\lambda} - (\omega_\lambda-\omega)\right),$$

$$\omega_\lambda = \frac{\hbar\lambda^2}{2m_c}. \quad (75)$$

The argument of the cosine in Eq. (71) contains the impact-ionization electro-optical frequency ω_F^{ii} and the (Fermi's golden rule) threshold $\mu^2\omega_{\rm th}$

$$\omega_F^{ii} = \left(\frac{1}{\mu}\frac{(e\mathcal{E})^2}{8m^*\hbar}\right)^{1/3}, \qquad \bar{\omega} = \omega_{\rm th} - [\omega_f(k)-\omega], \quad (76)$$

$$\omega_{\rm th} = \frac{1}{\mu^2}\frac{\hbar}{2m_c}k_{\rm th}^2, \quad k_{\rm th} = \sqrt{\frac{2m_c}{\hbar^2}\mu E_g}, \quad \mu = \frac{1+2\alpha}{1+\alpha}, \quad \alpha = \frac{m_c}{m_v}. \quad (77)$$

In Eq. (71) $\omega_{\max}$ expresses the energy width of the conduction band; it would be infinite for a purely parabolic semiconductor.

We shall now analyze Eq. (71) in the long-time Markov limit without neglect of the electric field. The summation over k_t in Eq. (71) allows one to substitute k_{t_+} with $k \equiv k_t$. As a consequence $f_e(k_{t'},t')$ becomes $f_e(k_{-t_-/2},t-t_-)$. Applying the Markov limit, the distribution function is taken out of the time integral and approximated by its value at t. Then we obtain

$$\frac{dn(t)}{dt} = \sum_k f_e(k,t)\int_0^{\omega_{\max}} d\omega\, S(\omega_f(k),\omega_f(k)-\omega) \times \frac{1}{\omega_F^{ii}}\int_0^{t-t_0} d\tau' \frac{1}{\pi}\cos\left(\frac{1}{3}\tau'^3 + \frac{\bar{\omega}}{\omega_F^{ii}}\tau'\right). \quad (78)$$

For $t_0 \to -\infty$ the time integration can be carried out yielding

$$\frac{dn(t)}{dt} = \sum_k f_e(k,t)\,P(k,\mathcal{E}),$$

$$P(k,\mathcal{E}) = \int_0^{\infty} d\omega\, S(\omega_f(k),\omega_f(k)-\omega)\,\frac{1}{\omega_F^{ii}}\mathrm{Ai}\left(\frac{\bar{\omega}}{\omega_F^{ii}}\right). \quad (79)$$

Here $\omega_{\max}$ is extended to infinity. This is possible due to the exponential decay of the Airy function Ai for positive arguments. By comparing the above expression with the corresponding rate of the Franz-Keldysh effect we see that $\omega_{\rm th}$ substitutes ω_g, and ω_f substitutes ω_L. The integration over ω here reflects the fact that, due to energy-time uncertainty, also energy-nonconserving transitions to higher energy states in the conduction band are possible, and corresponds to the summation over k in the derivation of the Franz-Keldysh formula. Here the integration over ω must be performed numerically.

In the limit of a vanishing electric field $\mathcal{E}$ Eq. (79) reduces to the semiclassical result obtained with Fermi's golden rule.[21,31] The scattering rate becomes

$$P(k,\mathcal{E}=0) = \int_0^{\infty} d\omega\, S(\omega_f(k),\omega_f(k)-\omega)\,\delta(\bar{\omega}) \equiv S(\omega_f(k),\omega_G), \quad \omega_f \geq \omega_G. \quad (80)$$

In Fig. 5 the impact-ionization scattering rate $P(k,\mathcal{E})$ is shown as a function of energy $E_c(k)$ for different val-

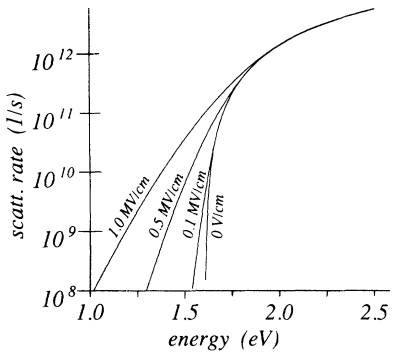

FIG. 5. Impact-ionization scattering rate $P(k,\mathcal{E})$ as a function of the energy $E_c(k) = \hbar^2k^2/(2m_c)$ for different values of the electric field $\mathcal{E}$, calculated for GaAs at $T = 300\,\mathrm{K}$.

ues of the applied electric field and compared with the zero-field limit, i.e., the semiclassical rate.[21,31] For the calculation we assumed GaAs with the same parameters as in Sec. IV A. It is clearly seen in the figure that the effective impact-ionization threshold is shifted to smaller values when an electric field is applied. This is a result of the intracollisional field effect by which virtually generated electron-hole pairs gain energy from the electric field during the impact-ionization scattering process.

VI. CONCLUSIONS

We have derived a closed set of quantum kinetic equations for the electron and hole distribution functions, the interband polarization, and the impact-ionization density-correlation functions which describe the coherent action of an external electric field in terms of Zener tunneling, field-assisted impact ionization, and Auger recombination. In the basis of accelerated Bloch waves, polarization-induced and impact-ionization-induced carrier generation processes with non-Markovian properties reflecting energy-time uncertainty arise. The first-order coherent contribution of impact ionization and Auger recombination renormalizes the carrier energies and the electric field. This extends and complements work in which electron-phonon and/or carrier-carrier scattering was considered in addition to the action of a constant external electric field[9] or a classical laser field,[14,32] but where processes that change the number of carriers in a band due to electron-electron interaction were neglected.

The theory of field-assisted impact ionization presented here differs substantially from earlier work.[6–8,16] We apply a full quantum transport theory based on the density-matrix formalism with the inclusion of distribution functions and the Pauli exclusion principle. We clarify the different effects of the electric field by splitting the electric field interaction $H_{\mathcal{E}}$ into accelerating ($H_{\|}$) and polarizing ($H_{\perp}$) components. Furthermore, our explicit calculations take full account of the q dependence of the Coulomb matrix element and thus go beyond the Keldysh approximation of $M_e(q)$ by its value at threshold. Our approach can be extended to the spatially inhomogeneous case, for example, by transforming to the Wigner representation.

In summary, we have shown that for strong electric fields quantum corrections lead to an enhanced generation of carriers by impact ionization and a softened effective impact-ionization threshold, as compared to the semiclassical theory. This is mathematically described by a smeared-out energy gap. The impact-ionization threshold is not a fixed field-independent quantity as it would result from the first-order perturbation theory (Fermi's golden rule) commonly used in semiclassical transport to describe incoherent transitions. The reason for this is the intracollisional field effect due to the intraband acceleration of carriers during the impact-ionization process even in the Markov limit. The derived analytical formulas make evident the close connection of field-assisted impact ionization with other field-assisted generation processes. In particular, the decrease of the effective impact-ionization threshold with field is the analog of the Franz-Keldysh effect in semiconductor optics.

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APPENDIX A: THE EQUATION OF MOTION

In this appendix we demonstrate that for a homogeneous electric field the effect of $H_{\|}$ can be removed from Heisenberg's equation of motion. Let us consider an arbitrary time-independent Schrödinger operator A and define

$$\tilde{A} := U_t(H_{\|})\, A\, U_t^{\dagger}(H_{\|})\,. \tag{A1}$$

The operator $\tilde{A}$ transformed into the Heisenberg picture ($\tilde{A}_H$) obeys the following equation of motion:

$$\frac{d}{dt}\tilde{A}_H = \frac{i}{\hbar}\left[(H - H_{\|}), \tilde{A}_H\right]\,. \tag{A2}$$

Let us illustrate the effect of Eq. (A2) for the electron distribution function f_e. In the spirit of Chambers' approach to semiclassical transport[33] we define the following function:

$$\tilde{f}_e(k_0,t) \equiv f_e(k_t,t)\,. \tag{A3}$$

Since the following identity holds:

$$c_{k_t} = U_t(H_{\|})\, c_{k_0}\, U_t^{\dagger}(H_{\|})\,, \tag{A4}$$

(and analogous ones for $c_k^{\dagger}$ and $c_k^{\dagger}c_k$), the function $\tilde{f}_e$ can be written as

$$\tilde{f}_e(k_0,t) = \left\langle U_t(H_{\|})\, c_{k_0}^{\dagger} c_{k_0}\, U_t^{\dagger}(H_{\|})\right\rangle\,, \tag{A5}$$

and according to Eq. (A2) $\tilde{f}_e$ obeys

$$\frac{d}{dt}\tilde{f}_e(k_0,t) = \frac{i}{\hbar}\left\langle[(H-H_{\|}),c^{\dagger}_{k_t}c_{k_t}]\right\rangle = \frac{d}{dt}f_e(k_t,t)\ . \tag{A6}$$

The drift term of the semiclassical Boltzmann equation is obtained by substituting in Eq. (A3) k_t with k

$$\left.\frac{d}{dt}\tilde{f}_e(k_0,t)\right|_{k_0=k+\frac{e\mathcal{E}}{\hbar}t} = \frac{\partial}{\partial t}f_e(k,t) - \frac{e\mathcal{E}}{\hbar}\frac{\partial}{\partial k}f_e(k,t)\ , \tag{A7}$$

or, equivalently,

$$\begin{aligned}\frac{d}{dt}f_e(k,t) &= \frac{\partial}{\partial t}f_e(k,t) - \frac{e\mathcal{E}}{\hbar}\frac{\partial}{\partial k}f_e(k,t)\\ &= \frac{i}{\hbar}\left\langle[(H-H_{\|}),c^{\dagger}_{k}c_{k}]\right\rangle\ .\end{aligned} \tag{A8}$$

The left-hand side of Eq. (A8) is equal to the left-hand side of Boltzmann's equation, the right-hand side has the meaning of the scattering contribution to the evolution of the distribution function. In contrast to Boltzmann's or Chambers' equation, Eqs. (A6) and (A8) are not closed but are only the first level of a coupled hierarchy of infinitely many differential equations for the expectation values of operator products.

APPENDIX B: FIELD-ASSISTED IMPACT IONIZATION IN SILICON

In this appendix we extend the theory of Sec. V B to the case of an indirect semiconductor to demonstrate that here besides phonon scattering also impact ionization is able to supply the necessary momentum for the Zener transition. We concentrate on silicon and, to describe the impact-ionization process with the lowest semiclassical threshold (see Fig. 6), need the following valence and conduction band dispersion relations (parabolic band approximation of silicon)

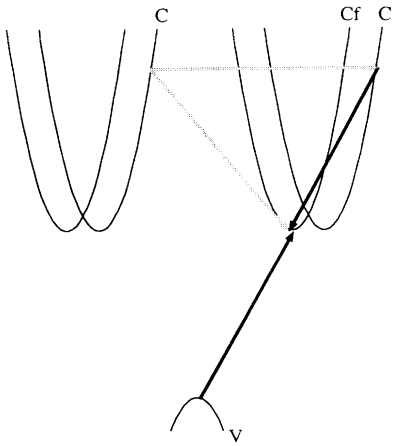

FIG. 6. Schematic impact-ionization transition in silicon with the lowest (semiclassical) threshold (umklapp process, denoted by shaded arrow).

$$E_c(k) = \frac{\hbar^2}{2m_c}\sum_i \beta_i k_i^2\ , \qquad m_c = (m_{c,1}\,m_{c,2}\,m_{c,3})^{1/3}\ ,$$

$$\beta_i = \frac{m_c}{m_{c,i}}\ , \tag{B1}$$

$$E_{cf}(k) = \frac{\hbar^2}{2m_c}\sum_{i=1}^{3}\beta_i(k_i - Z_{cf,i})^2\ , \tag{B2}$$

$$E_v(k) = E_{\rm gap} + \frac{\hbar^2}{2m_c}\sum_{i=1}^{3}\alpha(k_i - Z_{v,i})^2\ , \qquad \alpha = \frac{m_c}{m_v}\ . \tag{B3}$$

Here $E_c(k)$ describes the energy dispersion of the lowest parabolic (but not spherical) conduction band of silicon (X valley) and m_c is the effective conduction band mass, whose introduction will be useful later. $E_{cf}(k)$ expresses the same energy dispersion, but of the neighboring equivalent X valley and $E_v(k)$ describes the energy dispersion of the heavy-hole valence band in spherical parabolic band approximation. The zero of the energy scale coincides with the conduction band edge. The k-space origin is chosen to lie in the minimum of that X valley from which the impact-ionization process initiates. $Z_{v,i}$ and $Z_{cf,i}$ denote the k-space distance of the other respective band extrema.

With these energy dispersion relations again Eq. (71) is obtained but with the following different meaning of the parameters. First, the definition for the impact ionization mean free flight time τ is changed to

$$\frac{1}{\tau} = \frac{1}{\pi^2}\sqrt{\mu}\left(\prod_{i=1}^{3}(\alpha+\beta_i)^{-1/2}\right)\left(\frac{e^2|F_{vc}F_{cc}|\sqrt{m_c}}{\epsilon\epsilon_0\hbar^{3/2}}\right)^2\ . \tag{B4}$$

Second, the frequency associated with the energy of the impact-ionizing conduction electron ω_f is changed to

$$\omega_f(k^*) = \frac{1}{\mu^2}\frac{\hbar}{2m_c}\left[k^{*2}\left(\cos^2\theta + \frac{\mu_3\beta_2}{\mu_2\beta_3}\sin^2\theta\right) + (A+B)^2 - 2|A+B||k^*|\cos\theta\right], \tag{B5}$$

where $k_i^* = \sqrt{\beta_i}k_i$ (Herring-Vogt transformation) and θ is the angle between k^* and the electric field direction assumed antiparallel to k_3. The electro-optical frequency in this case becomes

$$\omega_F^{ii} = \left(\frac{\alpha+\beta_3}{\mu}\frac{(e\mathcal{E})^2}{8m_c\hbar}\right)^{1/3}\ , \tag{B6}$$

and $\omega_{\rm th}$ now depends on $|k^*|$

$$\omega_{\rm th}(k^*) = \frac{1}{\mu^2}\frac{\hbar}{2m_c}\left[k_{\rm th}^{*2} + (A+B)^2 + 2|B|k_{\rm th}^* - 2|A||k^*|\cos\theta\right]\ , \tag{B7}$$

where

$$k^*_{\rm th} = \sqrt{\mu_3 \left(\frac{2m_c E_g}{\beta_3 \hbar^2} + \frac{\alpha+\beta_3}{\alpha\beta_3} B^2 \right)} - B ,$$

and

$$\mu_i = \frac{\beta_i(\beta_i + 2\alpha_i)}{\alpha_i + \beta_i} , \quad \mu = \left(\prod_{i=1}^{3} \mu_i \right)^{1/3} . \tag{B8}$$

The constants A and B finally contain the information about the location in k space of the different band edges

$$A = \frac{1}{\sqrt{\beta_3}} \mu_3 Z_{cf,3} , \quad B = \frac{1}{\sqrt{\beta_3}} \frac{\alpha_3\beta_3}{\alpha_3+\beta_3} (Z_{v,3} - 2Z_{cf,3}) . \tag{B9}$$

The above expressions can be derived from a more general formula[31] if we assume the k_3 direction of the k-space coordinate system in the (001) direction of silicon and the electric field applied in the same direction.

With the above redefined parameters the formulas of Sec. V B remain valid. In Fig. 7 the impact-ionization scattering rate $P(k^*, \mathcal{E})$ of Eq. (79) for silicon is plotted as a function of energy $E_c(k^*)$. In the calculation the following values for silicon were assumed:

$$Z_v = (0, 0, 1.15\Delta) , \quad Z_{cf} = (0, 0, 0.3\Delta) , \tag{B10}$$

$$m_v = 0.6m_e , \quad m_{c,1} = m_{c,2} = 0.19m_e , \quad m_{c,3} = 0.98m_e , \tag{B11}$$

where $\Delta = 2\pi/a$ and $a = 5.43 \times 10^{-10} m$ is the lattice constant of silicon. Comparing the field-assisted impact-ionization rates in Si and in GaAs it is seen that the field effect in GaAs is much more drastic. This is due to several reasons. Even without field the impact-ionization threshold in Si is much softer than in GaAs since it is not isotropic.[13] Furthermore, the large momentum involved in transitions near threshold makes the Coulomb matrix element small. The most important reason, however, is the smaller electro-optical frequency in Si due to the large conduction band mass in the k_3 direction (direction with the smallest Fermi's golden rule threshold). An electron-hole pair state that is created with no energy support has an energy uncertainty of about the gap energy and can survive a corresponding time interval. During that lifetime in the same electric field an electron-hole pair in GaAs can gain much more energy than in Si due to the much smaller conduction band mass. This fact is reflected in the ratio $E_g/(\hbar\omega_F)$ which for an electric field of 10^6 V/cm is 12.6 in GaAs and 21.4 in Si.

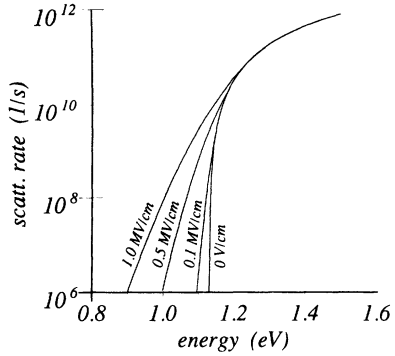

FIG. 7. Impact-ionization scattering rate $P(k^*, \mathcal{E})$ as a function of the energy $E_c(k^*)$ for different values of the electric field, calculated for Si.

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