Interband transition rate in GaAs

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Starting from a quantum-kinetic Boltzmann equation, the scattering rate for interband transition processes in GaAs is calculated numerically, taking into account a realistic band structure with corresponding Bloch wave functions. We compare with approximate solutions for this scattering rate such as the Keldysh or the Bethe formula, which are frequently used in simulations for high-field electron transport in solids. Based on the parameter-free numerical results, a fit formula for the impact ionization rate in GaAs is derived.

I. INTRODUCTION

The theoretical description of electronic transport, e.g., in semiconductor devices in the submicrometer range where very high electric fields can occur or in those operating on the basis of highly energetic (hot) electrons, requires knowledge about the high-field behavior of the electronic distribution. The electronic distribution function is usually determined from a quantum-kinetic transport equation that includes the different collision rates for, e.g., electron-electron, electron-phonon, and electron-impurity scattering in the respective collision term. The field heating of the electron distribution is generally balanced by inelastic phonon scattering processes that yield an average carrier energy and determine the shape of the nonequilibrium distribution function. Electrons from the high-energy tail are responsible for interband transition processes. Especially at very high electric fields, this process becomes effective in limiting the energy gain of the electrons due to the electric field and determines essentially the critical field strength of the so-called breakdown. Therefore, this scattering mechanism has to be treated rigorously for the case of quantum-kinetic transport in very high electric fields.

In this paper we will deal with the special problem of interband transitions in GaAs. There have been theories developed[1-6] with this topic that, however, contain adjustable parameters such as the threshold energy for ionization. An analytical solution for the impact ionization rate has not been in reach up to now, essentially because of two reasons. First, for the high-energy region that is relevant for interband transitions, a realistic band structure has to be considered. Second, the momentum-dependent interband transition matrix elements have to be determined using wave functions that are consistent with the band-structure calculations.

We have calculated numerically the interband transition rate in GaAs taking into account a pseudopotential band structure and the corresponding wave functions. We have applied a special integration method using special points,[7-9] to make this numerical problem tractable. Details of the calculation are given in Sec II. The numerical result for the interband transition rate is compared in Sec. III with different approximate solutions such as the Keldysh[2] or the Bethe formula,[10] which are frequently used in simulations of high-field transport in GaAs.[11,12] The results obtained from our numerical treatment of the problem indicate that the Keldysh formula is valid near the threshold energy and that the interband transition rate decreases for large energies, as predicted by the Bethe formula. We believe that our numerical results can give well-founded hints for the decision of a long-standing issue, namely whether a "soft" or a "hard" threshold is the relevant behavior for the interband transition rate, at least with respect to GaAs. In addition, we derive a simple fit formula for this scattering rate that may be used for calculations of the electron distribution function in GaAs for high electric fields, if all the other scattering mechanisms are also taken into account.

II. INTERBAND TRANSITION RATE

We will start with the quantum-kinetic Boltzmann equation for the electron distribution function $f_\nu(\mathbf{k},t)$,

$$\frac{\partial}{\partial t}f_\nu(\mathbf{k},t)+e\mathbf{E}\cdot\nabla_{\mathbf{k}}f_\nu(\mathbf{k},t)=I_{\mathrm{coll}}(\mathbf{k})\ , \tag{1}$$

where $\mathbf{E}$ is the electric-field strength. The collision term $I_{\mathrm{coll}}(\mathbf{k})$ is related to the self-energy, which is usually calculated by means of the Green's-function technique within the random-phase approximation,[13]

$$I_{\mathrm{coll}}(\mathbf{k}_1)=\frac{2\pi}{\hbar}\frac{\Omega^3}{(2\pi)^9}\sum_{\nu_2,\ldots,\nu_4}\int_{\mathrm{BZ}}\int_{\mathrm{BZ}}\int_{\mathrm{BZ}}d^3k_2d^3k_3d^3k_4|\langle\Psi^{\nu_1}_{\mathbf{k}_1}\Psi^{\nu_2}_{\mathbf{k}_2}|V(\mathbf{k}_1-\mathbf{k}_3)|\Psi^{\nu_3}_{\mathbf{k}_3}\Psi^{\nu_4}_{\mathbf{k}_4}\rangle|^2$$
$$\times\delta(E_{\nu_1}(\mathbf{k}_1)+E_{\nu_2}(\mathbf{k}_2)-E_{\nu_3}(\mathbf{k}_3)-E_{\nu_4}(\mathbf{k}_4))[f_{\nu_3}(\mathbf{k}_3)f_{\nu_4}(\mathbf{k}_4)-f_{\nu_1}(\mathbf{k}_1)f_{\nu_2}(\mathbf{k}_2)]\ . \tag{2}$$

The integrals are extended over the Brillouin zone, where Ω is the crystal volume, and $\Psi_{\mathbf{k}_i}^{\nu_i}, E_{\nu_i}(\mathbf{k}_i)$ denote wave function and energy of an electron with the wave vector $\mathbf{k}_i$ in the band ν_i, respectively. For interband transition processes, the initial states belong to the conduction (1) and valence band (2), whereas the final ones are conduction electron states [(3) and (4)]. $V(\mathbf{k})$ is the Coulomb potential and $f_\nu(\mathbf{k})$ the nonequilibrium distribution function. In the case of insulators and semiconductors with nearly empty conduction bands, we can simplify Eq. (2),

$$I_{\text{coll}}(\mathbf{k}_1)\approx I_{\text{coll}}(E)=-r(E)f_{\nu_1}(E)\ , \tag{3}$$

where

$$r(E)=\frac{2\pi}{\hbar}\frac{\Omega^3}{(2\pi)^9}\left[\sum_{\nu_1}\int_{\text{BZ}}d^3k_1\,\delta(E_{\nu_1}(\mathbf{k}_1)-E)\right]^{-1}$$
$$\times\sum_{\nu_1,\ldots,\nu_4}\int_{\text{BZ}}\cdots\int_{\text{BZ}}d^3k_1d^3k_2d^3k_3d^3k_4\,|\langle\Psi_{\mathbf{k}_1}^{\nu_1}\Psi_{\mathbf{k}_2}^{\nu_2}|V(\mathbf{k}_1-\mathbf{k}_3)|\Psi_{\mathbf{k}_3}^{\nu_3}\Psi_{\mathbf{k}_4}^{k_4}\rangle|^2$$
$$\times\delta(E_{\nu_1}(\mathbf{k}_1)-E)\delta(E_{\nu_1}(\mathbf{k}_1)+E_{\nu_2}(\mathbf{k}_2)-E_{\nu_3}(\mathbf{k}_3)-E_{\nu_4}(\mathbf{k}_4))\ , \tag{4}$$

denotes the interband transition rate averaged over all directions in $\mathbf{k}$ space. Equation (4) was solved by Keldysh[2] expanding the integrand near the threshold energy and neglecting the dependence of the matrix elements on the momenta $\mathbf{k}_3,\mathbf{k}_4$ of the final states. Baraff[4] developed a theoretical approach to the field dependence of the ionization rate, which yields the results of Wolff[1] and Shockley[3] in the limiting cases of high and low fields, respectively. However, this theory contains several adjustable parameters such as the threshold energy or the phonon scattering rate for best fitting the experimental ionization coefficients.

Kane[14] solved Eq. (4) within the constant matrix approximation allowing for exchange processes and considering a realistic band structure as well as the dielectric function $\epsilon(q,\omega)$ for Si. The remaining integrals over δ functions were evaluated by a Monte Carlo method. Geist and Gladden[15] supposed a parabolic band structure for Si and they could then solve most of the integrations in Eq. (4) analytically. Their results indicated only small modifications of the ionization rate for energies between the threshold and the plasmon energy compared to that of Kane.

We have done a full numerical calculation of $r(E)$ for GaAs using the band structure and the matrix elements corresponding to the true electron wave functions. The interband transition rate obtained numerically is compared to the usual Keldysh[2] and Bethe formula[10] and, furthermore, to the results of an approximately parabolic band structure. The contribution to the transition rate resulting from umklapp processes will also be investigated.

A. Numerical treatment

A pseudopotential calculation[16,17] yields the energy eigenvalues in the different bands $E_\nu(\mathbf{k})$ and the corresponding eigenfunctions as a plane-wave expansion with the coefficients $\alpha_{\mathbf{G}}^{(\nu)}(\mathbf{k})$,

$$\Psi_{\mathbf{k}}^{\nu}(\mathbf{r})=\frac{1}{\sqrt{\Omega}}e^{i\mathbf{k}\cdot\mathbf{r}}u_{\nu\mathbf{k}}(\mathbf{r})=\frac{1}{\sqrt{\Omega}}\sum_{\mathbf{G}}\alpha_{\mathbf{G}}^{(\nu)}(\mathbf{k})e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}\ , \tag{5}$$

where $u_{\nu\mathbf{k}}(\mathbf{r})$ are the Bloch factors. The $\mathbf{G}$'s range is four or six shells in the reciprocal lattice, which means $|\mathbf{G}|^2\le 8(2\pi/a)^2$ or $|\mathbf{G}|^2\le 12(2\pi/a)^2$, where a is the lattice constant. A screened electron-electron interaction potential in the Born approximation,

$$V(\mathbf{q})=\frac{e^2}{\epsilon_0}\frac{1}{\mathbf{q}^2+\kappa^2}\ ,$$
$$\kappa^2=\frac{m_e e^2}{\pi\epsilon\epsilon_0\hbar^2}\left[\frac{3n_e}{\pi}\right]^{1/3},\quad \epsilon=12.9\ , \tag{6}$$

with n_e being the valence-electron density of GaAs, leads to the following representation for the matrix element in (4):

$$|\langle\Psi_{\mathbf{k}_1}^{\nu_1}\Psi_{\mathbf{k}_2}^{\nu_2}|V(\mathbf{k}_1-\mathbf{k}_3)|\Psi_{\mathbf{k}_3}^{\nu_3}\Psi_{\mathbf{k}_4}^{\nu_4}\rangle|^2=\frac{1}{\Omega^2}\left[\frac{e^2}{\epsilon_0}\right]^2\sum_{\mathbf{K}'}\left|\sum_{\mathbf{K}}\frac{1}{|\mathbf{K}+\mathbf{k}_1-\mathbf{k}_3|^2+\kappa^2}B_{\nu_1\nu_3}^{(\mathbf{K})}(\mathbf{k}_1,\mathbf{k}_3)B_{\nu_2\nu_4}^{(\mathbf{K}'-\mathbf{K})}(\mathbf{k}_2,\mathbf{k}_4)\right|^2\delta_{\mathbf{K}',\mathbf{k}_3+\mathbf{k}_4-\mathbf{k}_1-\mathbf{k}_2}\ . \tag{7}$$

The Bloch integrals are given by

$$B_{\nu\nu'}^{(\mathbf{K})}(\mathbf{k},\mathbf{k}')=\frac{1}{\Omega}\int d^3r\,e^{i\mathbf{K}\cdot\mathbf{r}}u_{\nu\mathbf{k}}^*(\mathbf{r})u_{\nu'\mathbf{k}'}(\mathbf{r})\ . \tag{8}$$

After integrating over the momentum δ function, the transition rate, Eq. (4), can be written as

$$r(E)=\frac{2\pi}{\hbar}\frac{1}{(2\pi)^6}\left[\sum_{\nu_1}\int_{\mathrm{BZ}}d^3k_1\,\delta(E_{\nu_1}(\mathbf{k}_1)-E)\right]^{-1}$$
$$\times\sum_{\nu_1,\ldots,\nu_4}\int_{\mathrm{BZ}}\int_{\mathrm{BZ}}\int_{\mathrm{BZ}}d^3k_1\,d^3k_3\,d^3k_4$$
$$\times\delta(E_{\nu_1}(\mathbf{k}_1)-E)\,\delta(E_{\nu_1}(\mathbf{k}_1)+E_{\nu_2}(\mathbf{k}_3+\mathbf{k}_4-\mathbf{k}_1)-E_{\nu_3}(\mathbf{k}_3)-E_{\nu_4}(\mathbf{k}_4))$$
$$\times\left[\frac{e^2}{\epsilon_0}\right]^2\left|\sum_{\mathbf{K}}\frac{1}{|\mathbf{K}+\mathbf{k}_1-\mathbf{k}_3|^2+\kappa^2}B^{(\mathbf{K})}_{\nu_1\nu_3}(\mathbf{k}_1,\mathbf{k}_3)B^{(-\mathbf{K})}_{\nu_2\nu_4}(\mathbf{k}_3+\mathbf{k}_4-\mathbf{k}_1,\mathbf{k}_4)\right|^2 . \tag{9}$$

The sums over the band indexes ν_1,ν_3,ν_4 each involve the first 27 or 59 conduction bands, whereas the ν_2 sum runs over the four valence bands of GaAs. Umklapp processes are described by additional contributions due to the reciprocal-lattice vector $\mathbf{K}$ in the matrix element [Eq. (7)]. In the case of $|\mathbf{K}|=0$ we have normal processes. Our considerations will be restricted to normal processes and umklapp processes up to third order.

The ninefold integration in Eq. (9) is treated numerically using a special point method.[7–9] Then each integration over the Brillouin zone is approximated by a weighted sum over values of the integrand at special points $\mathbf{k}_i$ according to

$$\frac{\Omega_0}{(2\pi)^3}\int_{\mathrm{BZ}}d^3k f(\mathbf{k})=\frac{1}{n}\sum_{P_j}\sum_{\mathbf{k}_i}\beta_i f(P_j\mathbf{k}_i) , \tag{10}$$

with the normalization condition for the weighting factors β_i

$$\sum_i\beta_i=1,\quad \beta_i>0 .$$

Ω_0 is the volume of the primitive cell. If $f(\mathbf{k})$ does not fulfill the symmetric properties of the respective lattice point group, the sum must be extended over all n symmetry operations P_j of this group. In order to make a numerical treatment possible, we approximate both energy δ functions in Eq. (9) as Lorentz profiles like

$$\delta(x)\approx\frac{1}{\pi}\frac{\eta}{x^2+\eta^2} .$$

The special choice of the parameter η does not essentially affect the results. We take $\eta=0.2$ eV in accordance with Kane,[14] who replaced the δ functions by rectangles of unit area and width of 0.1 eV for primary energy and 0.4 eV for energy conservation, so that the energy conservation was satisfied to within 0.2 eV.

B. Approximate solutions

Two alternative analytical formulas for impact ionization are well known. The Keldysh formula[2] results from an expansion of the integrand of Eq. (4) near the threshold. Therefore a reasonable description of the ionization process in the case of higher energies cannot be expected. Keldysh obtained the following "soft" threshold behavior:

$$r(E)=\begin{cases}0, & E<E_{\mathrm{th}}\\ C\left[\dfrac{E-E_{\mathrm{th}}}{E_{\mathrm{th}}}\right]^2, & E\geq E_{\mathrm{th}} .\end{cases} \tag{11a}$$

The parameter $C=1.19\times10^{14}\ \mathrm{s}^{-1}$ can be determined by a straightforward application of Keldysh's approximation. The threshold energy was calculated within the parabolic band approximation analytically, taking the Fermi energy at the top of the valence band,

$$E_{\mathrm{th}}=\frac{3-2m_v^*/m_c^*}{1-m_v^*/m_c^*}E_g .$$

We consider the upper three valence bands by calculating the contribution of each band with its effective mass and, therefore, its corresponding threshold energy. For the effective masses of the valence bands we take $m^*_{v_{1,2}}=-0.68m_e$ and $m^*_{v_3}=-0.12m_e$, whereas $m_c^*=0.07m_e$ is the conduction electron mass. The value of $E_g=1.36$ eV was obtained from the band-structure calculation.

Alternatively a Bethe-like formula[10] for the transition rate,

$$r(E)=\begin{cases}0, & E<E_{\mathrm{th}}\\ \dfrac{B}{E}\ln\left[\dfrac{E}{E_{\mathrm{th}}}\right], & E\geq E_{\mathrm{th}}\end{cases} \tag{11b}$$

is used,[18] which represents a "hard" threshold behavior and where the fit parameter $B=2.5\times10^{16}$ eV/s gives the magnitude of the transition rate. Because this formula was evaluated by means of the Born approximation, it seems to be more appropriate in the range of higher energies. The threshold energy was determined in the just-mentioned way using the effective mass of the uppermost valence band.

A further approximate calculation of the interband transition rate [Eq. (4)] has been carried out within the framework of Geist and Gladden[15] applying the parabolic band model. The matrix element was treated by considering not only its dependence on the initial electron energy but taking into account the full $\mathbf{k}$ dependence of the interaction described by a screened Coulomb potential (see Sec. II A). In the free-electron approximation the Bloch integrals were rewritten as $\delta_{\mathbf{K},0}$. After a straightforward calculation we got two remaining integrals which were solved numerically. Similar to the treatment

of the Keldysh formula, we include the contributions of the three upper valence bands to the transition rate within the effective-mass approximation.

III. RESULTS

The special point method,[7–9] which was applied for the evaluation of the ninefold integration in Eq. (9), allows a totally numerical treatment of the problem. However, due to the limited computer time, we have to restrict to point sets including only a few points. We have investigated the convergence of this method with respect to a systematic increase of the point sets. Furthermore, the number of shells considered within the band-structure calculation limits the energy region where the band structure is described correctly. For the investigation of the high-energy behavior of the interband transition rate, we have therefore extended the number of shells for the band-structure calculation systematically. For instance, a four-shell calculation seems to be appropriate for energies $E \leq 18$ eV, whereas a six-shell calculation is needed to go up to $E \leq 30$ eV. In Fig. 1, we have shown the interband transition rates resulting from a one- up to a four-point scheme. Schemes with a higher number of special points soon require computer time beyond the scope of actual computer capacities. For instance, for each point in Fig. 1 within the one-point set and a four-shell band-structure calculation, we need 4-min cpu time on a CONVEX 120 supercomputer, whereas the four-point set combined with the six-shell band-structure calculation requires already 160-min cpu time. However, the convergence of the method is quiet satisfactory for our purposes.

The statistical scatter inherent in the curves for the transition rate, especially for energies higher than 10 eV, is due to the numerical algorithm; i.e., it depends on the choice of the special point set. We could not find any correlation between the "peaks" and the band structure. For energies lower than 10 eV a good agreement between the results of the different point sets can be pointed out. The threshold energy obtained from the one-point set[7] is too large by a factor of 3 because the Γ point is not included.

In Fig. 2 we compare our numerical results with different approximate solutions for the interband transition rate. For the low-energy range, i.e., near the threshold, our results coincide with the Keldysh formula[2] which was derived within a low-energy expansion near the threshold and using the matrix elements of Eq. (4) in the Born approximation and thus neglecting their dependence on the momenta $\mathbf{k}_3, \mathbf{k}_4$ of the final states. Therefore, we conclude that the interband transition rate in GaAs shows a "soft"-threshold behavior and that the correct calculation of the matrix element is of minor importance.

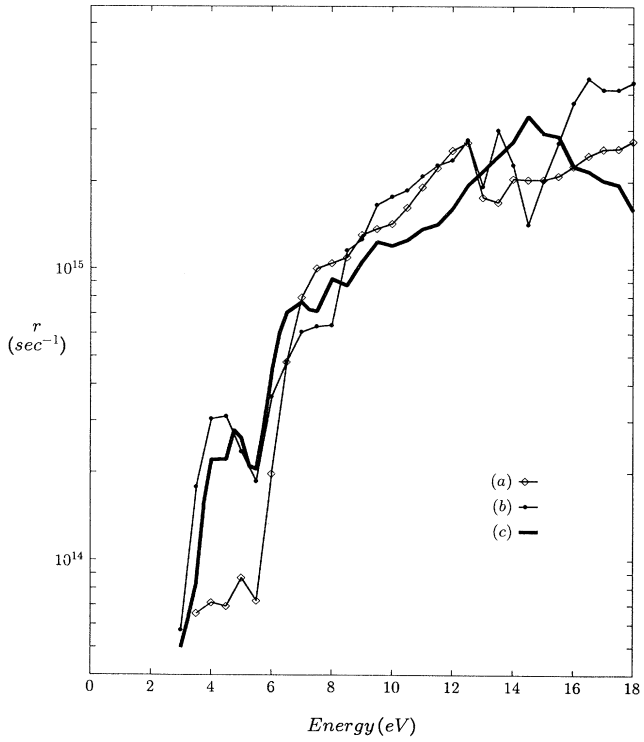

FIG. 1. Interband transition rate calculated numerically using (a) the one-point set (Ref. 7), (b) the two-point set (Ref. 8), and (c) the four-point set (Ref. 9).

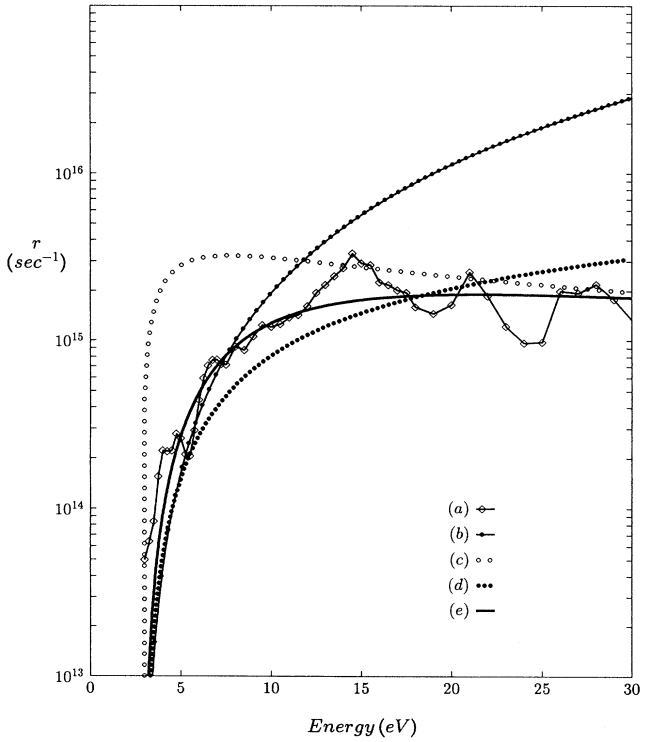

FIG. 2. Interband transition rate for GaAs calculated (a) numerically using the four-point set (Ref. 9), (b) using the Keldysh formula [Eq. (11a)], (c) using the Bethe formula [Eq. (11b)], (d) using the parabolic band approximation, and (e) using our fit formula [Eq. (12)].

The latter statement is underlined by comparing with the parabolic band approximation introduced in Sec. II B. In spite of the simple assumptions, however, the agreement with the numerical results and the Keldysh formula is very good, in accordance with the results of Kane[14] and Geist and Gladden.[15] Furthermore, the influence of higher bands can be neglected in this low-energy range, as one would expect.

The numerical results indicate that in the high-energy region ($E > 20$ eV) the Bethe formula[10] yields the correct asymptotic behavior for impact ionization. On the basis of these findings, we propose a simple fit formula for the interband transition rate which interpolates between the two analytically known cases for energies near the threshold and for high energies:

$$r(E)=\begin{cases} 0, & E < E_{\mathrm{th}} \\ C\dfrac{E-E_{\mathrm{th}}}{E_{\mathrm{th}}\left[1+AE^2/E_{\mathrm{th}}^2\right]}\ln\dfrac{E}{E_{\mathrm{th}}}, & E \geq E_{\mathrm{th}} \end{cases} . \tag{12}$$

For the threshold energy we take $E_{\mathrm{th}}=2.85$ eV (see Sec. II B). This fit shows a good overall agreement with the numerical results. For the parameter A we choose 0.08 to get the Bethe-like behavior for high energies. The prefactor $C=8\times10^{14}\ \mathrm{s}^{-1}$ is of the order of the proportionality constant, which can be extracted from the original paper of Keldysh. This prefactor is usually treated as a fit parameter and often identified with the optical-phonon scattering rate at the threshold energy,[11,12]

$$C=\frac{P}{\tau_{\mathrm{opt}}(E_{\mathrm{th}})} ,$$

where P is an arbitrary parameter which may simulate both a soft threshold (low P, low E_{th}) or a hard threshold (large P, large E_{th}). The choice of a large P together with an optical-phonon scattering rate of $[\tau_{\mathrm{opt}}(E_{\mathrm{th}})]^{-1} \approx 3\times10^{14}\ \mathrm{s}^{-1}$ as in Refs. 11 and 12 yields a hard threshold as well as impact ionization rates much greater than $10^{15}\ \mathrm{s}^{-1}$ near the threshold, both in contradiction to our numerical results.

We have also investigated the influence of umklapp processes up to third order in an extra calculation. The inclusion of umklapp processes yields ionization rates which are three to four times higher and the respective curves show the same shape as discussed before. The corresponding fit parameters for Eq. (12) are then $A=0.03$ and $C=2\times10^{15}\ \mathrm{s}^{-1}$. Therefore, umklapp processes have to be included when dealing with the complete interaction of electrons in solids at high fields.

IV. SUMMARY

The interband transition rate for GaAs was obtained from a numerical evaluation of Fermi's golden rule, neglecting the coupling with phonon processes. A pseudopotential band structure was considered for both energy conservation and matrix elements. We obtain sufficient convergence of the numerical procedure. The results show a Keldysh-like, soft-threshold behavior for the ionization rate at low energies, and a Bethe-like decrease at higher energies. The intermediate regime interpolates with some scatter at variance with the approximate integration scheme. Based on this behavior, a simple fit formula is proposed connecting the two asymptotic, analytically known results that may be used for future calculations of the nonequilibrium electron distribution function in GaAs. Then, from an improved understanding of the competing scattering processes in semiconductors such as electron-phonon scattering or impact ionization, additional insight into the high-field behavior of electronic transport may be gained.

Our procedure can immediately be generalized to allow for exchange processes in the matrix elements and for screening effects beyond the static limit chosen here. Furthermore, avoiding the average over the incident momentum $\mathbf{k}_1$ in Eq. (4), the orientation dependence of the interband transition rate can be investigated, which was experimentally observed for GaAs (Ref. 19) and Si.[20] Especially, the wave-vector dependence of the ionization threshold, which was found to play a major role in high-field transport in Si (Ref. 21), may be of some importance in GaAs, too.

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