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Gauge-invariant formulation of high-field transport in semiconductors

Emanuele Ciancio,* Rita C. Iotti,† and Fausto Rossi‡
Istituto Nazionale per la Fisica della Materia (INFM) and Dipartimento di Fisica, Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 Torino, Italy

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In this paper we revisit the conventional description of carrier-phonon scattering in the presence of high electric fields by means of a gauge-invariant density-matrix approach. The proposed formulation of the transport problem allows us, on the one hand, to provide a gauge-independent formulation of Fermi's golden rule; on the other hand, our analysis clearly shows that in the standard treatments of high-field carrier-phonon scattering—also referred to as intracollisional field effect—the possible variation of the basis states has been usually neglected. This is recognized to be the origin of the apparent discrepancy between scalar- and vector-potential treatments of the problem; indeed, a proper account of such contributions leads, in general, to an ill-defined Markov limit in the carrier-phonon interaction process, assigning to the scalar-potential or Wannier-Stark picture a privileged role. The neglect of such Zener-like contributions in the transport equation leads to a wrong estimation of the high-field voltage-current characteristics, and may partially account for the surprisingly good agreement between semiclassical and rigorous quantum-transport calculations previously reported. This is confirmed by fully three-dimensional simulations of charge transport in state-of-the-art semiconductor superlattices, which show a significant current overestimation.

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I. INTRODUCTION

Since the early days of quantum mechanics[1] the field-induced coherent dynamics of an electron wave packet within a crystal, known as *Bloch oscillations* (BO), has attracted significant and increasing interest.[2] Indeed, the problem of properly describing the scattering-free motion of an electron in a solid has led to a three-decade controversy on the existence of BO.[3] This originated from the different approaches employed for the description of the applied field, namely *the vector potential or accelerated-Bloch-state picture*[4] and *the scalar potential or Wannier-Stark description*.[5] As discussed in Ref. 6, these two pictures are now recognized to be fully equivalent, since they correspond to different quantum-mechanical representations connected by a gauge transformation.

The presence of scattering as well as tunneling processes strongly modifies such ideal BO scenario.[7] In particular, nonelastic interaction mechanisms—such as carrier-LO phonon scattering—tend to spoil such coherent dynamics, leading to a nearly semiclassical or Boltzmann-like transport picture. In the presence of strong electric fields, however, the use of the conventional scattering picture—involving transitions between field-free Bloch states within Fermi's golden rule—becomes questionable.

As originally pointed out by Levinson[8] and by Barker and Ferry,[9] the effect of the field during the scattering process, usually referred to as *intracollisional field effect* (ICFE), may lead to significant deviations from the semiclassical scenario. On the one hand, the role played by the ICFE has been extensively investigated by means of rigorous quantum-transport approaches.[10–13] Their application, however, was often limited to highly simplified physical models and conditions, thus preventing any quantitative comparison with experiments. On the other hand, strong effort has been devoted to incorporate the ICFE within conventional—and more realistic—Monte Carlo simulations.[14] In this case, the basic idea is that, due to the field-induced carrier drift, energy conservation in the scattering process is relaxed; as a consequence, the δ function of Fermi's golden rule is replaced by broad spectral functions.[15] We stress that this scenario, intimately related to the vector potential or accelerated picture, has no counterpart in the scalar-potential one. Indeed, within the Wannier-Stark basis there is no carrier drift, and energy conservation is preserved. It is thus clear that such an effective semiclassical description of the ICFE is not gauge invariant.[16] The aim of the present investigation is to explain and remove this apparent contradiction by providing a gauge-invariant formulation of Fermi's golden rule.

The paper is organized as follows: In Sec. II we shall introduce and discuss our gauge-invariant treatment of quantum-transport phenomena based on the single-particle density-matrix formalism; Sec. III will present a few simulated experiments aimed at comparing the proposed gauge-invariant formalism with conventional ICFE treatments; finally, in Sec. IV we shall summarize and draw some conclusions.

II. THEORETICAL APPROACH

A. Physical system

In order to describe quantum-transport phenomena in solids, and in particular in semiconductor nanostructures, let us consider a generic electron-phonon system, whose Hamiltonian can be schematically written as

$$\mathbf{H}=\mathbf{H}_o+\mathbf{H}'=(\mathbf{H}_c+\mathbf{H}_p)+\mathbf{H}_{cp}\,. \tag{1}$$

Within an ideal Schrödinger-equation treatment of the global electron-phonon problem, the above Hamiltonian dictates the motion of electrons and ions in the crystal. It can be regarded

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as the sum of a free-particle term $\mathbf{H}_o$ and of an interaction term $\mathbf{H}'$. More specifically, the system Hamiltonian includes the following contributions.

(i) The noninteracting carrier Hamiltonian

$$\mathbf{H}_c = \frac{\left(-i\hbar\nabla_{\mathbf{r}} - \frac{e}{c}\mathbf{A}(\mathbf{r},t)\right)^2}{2m_o} + e\varphi(\mathbf{r},t) + V^l(\mathbf{r}). \tag{2}$$

(ii) The free-phonon term

$$\mathbf{H}_p = \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}}. \tag{3}$$

(iii) The carrier-phonon coupling

$$\mathbf{H}_{cp} = \sum_{\mathbf{q}} \gamma_{\mathbf{q}}[b_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} + b_{\mathbf{q}}^\dagger e^{-i\mathbf{q}\cdot\mathbf{r}}]. \tag{4}$$

The Hamiltonian $\mathbf{H}_c$ describes noninteracting electrons within the effective lattice potential V^l interacting with a classical electromagnetic field expressed in terms of corresponding scalar and vector potentials φ and $\mathbf{A}$. The latter can be chosen in infinitely different ways; this is the so-called gauge freedom: it implies that the electromagnetic potentials must be chosen together with an external condition which fixes the gauge. When possible, two privileged gauge choices are considered, those resulting in a single electromagnetic potential, i.e., a vector or a scalar one (see below). For the case of a homogeneous static electric field $\mathbf{F}$ (and no magnetic field) this can be achieved by the following gauge transform:

$$\varphi_\eta(\mathbf{r}) = \varphi_0(\mathbf{r}) - \frac{1}{c}\frac{\partial}{\partial t} f_\eta(\mathbf{r},t),$$

$$\mathbf{A}_\eta(t) = \mathbf{A}_0(t) + \nabla f_\eta(\mathbf{r},t), \tag{5}$$

with $\varphi_0(\mathbf{r}) = -\mathbf{F}\cdot\mathbf{r}$, $\mathbf{A}_0(t) = 0$, and with the gauge function

$$f_\eta(\mathbf{r},t) = -\eta c\mathbf{F}\cdot\mathbf{r}t. \tag{6}$$

Here η is the free parameter of our gauge transformation. Indeed, more generally we have

$$\varphi_\eta(\mathbf{r}) = \varphi_{\bar\eta}(\mathbf{r}) - \frac{1}{c}\frac{\partial}{\partial t} f_{\eta-\bar\eta}(\mathbf{r},t),$$

$$\mathbf{A}_\eta(t) = \mathbf{A}_{\bar\eta}(t) + \nabla f_{\eta-\bar\eta}(\mathbf{r},t), \tag{7}$$

which for $\bar\eta = 0$ reduces to the gauge transformation in Eq. (5).

The explicit form of the scalar and vector potentials in Eq. (5) describing our constant and homogeneous field $\mathbf{F}$ is then given by

$$\varphi_\eta(\mathbf{r}) = -(1-\eta)\mathbf{F}\cdot\mathbf{r} = (1-\eta)\varphi_0(\mathbf{r}),$$

$$\mathbf{A}_\eta(t) = -\eta c\mathbf{F}t = \eta\mathbf{A}_1(t). \tag{8}$$

As we can see, the scalar-potential gauge is obtained by setting $\eta = 0$, while the vector-potential one corresponds to $\eta = 1$. The Hamiltonian expressed in terms of a single potential is quite useful since it can be easily diagonalized.

By inserting the explicit form of the electromagnetic potentials in Eq. (8) into the single-particle Hamiltonian $\mathbf{H}_c$, we finally get

$$\mathbf{H}_c = \frac{(-i\hbar\nabla_{\mathbf{r}} + \eta e\mathbf{F}t)^2}{2m_o} - (1-\eta)e\mathbf{F}\cdot\mathbf{r} + V^l(\mathbf{r}), \tag{9}$$

where, as anticipated, the gauge freedom is expressed in terms of the parameter η.[17,18]

The term $\mathbf{H}_p$ in Eq. (3) describes the free-phonon system via the second quantization creation and destruction operators $b_{\mathbf{q}}^\dagger$ and $b_{\mathbf{q}}$, $\omega_{\mathbf{q}}$ denoting the corresponding frequency-momentum dispersion relation.

Let us finally consider the interaction Hamiltonian $\mathbf{H}_{cp}$ in Eq. (4). It describes the coupling between electrons and bulk phonons. Here, the explicit form of the coupling function $\gamma_{\mathbf{q}}$ depends on the particular interaction mechanism considered, e.g., deformation potential, Frölich coupling, etc.

B. Density-matrix formalism

Following the general prescription of the time-dependent perturbation theory, we start by looking for a suitable, complete orthonormal set which diagonalizes the free-carrier Hamiltonian. The corresponding eigenvalue equation reads

$$\mathbf{H}_c\phi_\alpha(\mathbf{r}) = \epsilon_\alpha\phi_\alpha(\mathbf{r}). \tag{10}$$

Our basis states are then the eigenstates of $\mathbf{H}_c$ in Eq. (9), which of course depend on the gauge choice. Therefore, in general, we deal with different sets of eigenstates, according to the value of the parameter η. As anticipated, the two particular cases $\eta = 0$ and $\eta = 1$ involve, respectively, the scalar and the vector potential only. In general, the quantum numbers α—and therefore the corresponding eigenfunctions $\phi_\alpha(\mathbf{r}) \equiv \langle\mathbf{r}|\alpha\rangle$ and energies ϵ_α—are functions of the transformation parameter η, and for $\eta \neq 0$ are also time dependent.[19]

For $\eta = 0$ (scalar-potential gauge) we recover the well-known Wannier-Stark states:[5]

$$\phi_\alpha(\mathbf{r}) = \phi_{\mathbf{k}_\perp n,\nu}(\mathbf{r}), \quad \epsilon_\alpha = \epsilon_{\mathbf{k}_\perp n,\nu} \equiv \epsilon_{\mathbf{k}_\perp 0,\nu} + n\Delta\epsilon, \tag{11}$$

with $\Delta\epsilon = eFd$, d denoting the crystal periodicity along the field direction. As we can see, for any value of the carrier wave vector perpendicular to the field direction $\mathbf{k}_\perp$ and for any band-index value ν, we deal with a discrete and equally spaced energy spectrum, known as Wannier-Stark ladder. In the limit $F \to 0$ the Wannier-Stark states in Eq. (11) reduce to the usual Bloch states: $\phi_{\mathbf{k}_\perp n,\nu}(\mathbf{r}) \to \phi^o_{\mathbf{k}\nu}(\mathbf{r})$, $\epsilon_{\mathbf{k}_\perp n,\nu} \to \epsilon^o_{\mathbf{k}\nu}$.

In contrast, for $\eta = 1$ we deal with the Houston or accelerated Bloch states:[4]

$$\phi_\alpha(\mathbf{r},t) = \phi^o_{\mathbf{k}\nu}(\mathbf{r}) e^{(ie/\hbar)\mathbf{F}\cdot\mathbf{r}t} \tag{12}$$

with $\epsilon_\alpha = \epsilon^0_{\mathbf{k}(t)\nu}$, where $\mathbf{k}(t) = \mathbf{k}_0 + \dot{\mathbf{k}}t$ is the instantaneous carrier wave vector, $\dot{\mathbf{k}} = e\mathbf{F}/\hbar$ being its field-induced time variation. Again, in the limit $F \to 0$ the usual Bloch states are recovered.

In the first case ($\eta = 0$) we deal with the discrete quantum number n along the field direction, while in the second case ($\eta = 1$) we deal with the continuous index $k_\parallel$. We finally stress that the scalar-potential hamiltonian is time independent (but space dependent), while the vector-potential one is time dependent (but space independent).[6]

In general, the two basis states, corresponding to the two arbitrary gauge choices η and $\bar{\eta}$ in Eq. (7), will be connected by the following unitary transformation:

$$|\alpha(\eta)\rangle = \mathcal{U}^{\eta,\bar{\eta}}|\alpha(\bar{\eta})\rangle. \tag{13}$$

Given such basis states $\{|\alpha\rangle\}$, most of the physical quantities we are interested in—e.g., carrier drift velocity and mean kinetic energy—are properly described by the well-known single-particle density matrix[20]

$$\rho_{\alpha_1\alpha_2} = \langle a^\dagger_{\alpha_2} a_{\alpha_1}\rangle, \tag{14}$$

where $a^\dagger_\alpha$ (a_α) denotes creation (destruction) operator for a carrier in state α.[21] It is easy to show that the density matrix (14) will gauge transform according to

$$\rho^\eta_{\alpha_1\alpha_2} = \sum_{\bar{\alpha}_3\bar{\alpha}_4} U_{\bar{\alpha}_1\bar{\alpha}_3}\rho^{\bar{\eta}}_{\bar{\alpha}_3\bar{\alpha}_4} U_{\bar{\alpha}_4\bar{\alpha}_2}, \tag{15}$$

where $U_{\bar{\alpha}\bar{\alpha}'} = \langle\alpha|\bar{\alpha}'\rangle = \langle\bar{\alpha}|\mathcal{U}^{\bar{\eta},\eta}|\bar{\alpha}'\rangle$ are the matrix elements of $\mathcal{U}^{\bar{\eta},\eta}$ in the $\bar{\eta}$ representation. Here, the compact notation $\bar{\alpha} \equiv \alpha(\bar{\eta})$ has been introduced.

In the Heisenberg picture the time evolution of the single-particle density matrix (14) is dictated by the time evolution of the creation and destruction operators $a^\dagger_\alpha$ and a_α. For a time-dependent basis set $\{|\alpha\rangle\}$, we have[20]

$$\frac{d}{dt}a_\alpha = \frac{d}{dt}a_\alpha\bigg|_{\mathbf{H}} + \frac{d}{dt}a_\alpha\bigg|_{\phi}. \tag{16}$$

Compared to the standard equations of motion, the possible time variation of our basis states ϕ_α gives rise to an additional term; the latter is absent only if the single-particle Hamiltonian is time independent, i.e., in the scalar-potential gauge. When present, this extra term gives rise to nondiagonal matrix elements in the self-energy operator. These are known as Zener contributions. The explicit form of the two contributions on the right-hand side of Eq. (16) can be readily obtained by combining the standard Heisenberg equation of motion for the field operator,

$$\Psi(\mathbf{r}) = \sum_\alpha a_\alpha \phi_\alpha(\mathbf{r}), \tag{17}$$

with the explicit form of the creation/destruction operators, i.e.,

$$a_\alpha = \int d\mathbf{r}\phi^*(\mathbf{r})\Psi(\mathbf{r}). \tag{18}$$

More specifically, we get

$$\begin{aligned}\frac{d}{dt}a_\alpha &= \int d\mathbf{r}\left[\frac{d}{dt}\phi^*_\alpha(\mathbf{r})\right]\sum_{\alpha'}\phi_{\alpha'}(\mathbf{r})a_{\alpha'} \\ &\quad + \int d\mathbf{r}\phi^*_\alpha(\mathbf{r})\frac{1}{i\hbar}\left[\sum_{\alpha'}\phi_{\alpha'}(\mathbf{r})a_{\alpha'},\mathbf{H}\right] \\ &= \sum_{\alpha'}\int d\mathbf{r}\left[\frac{d}{dt}\phi^*_\alpha(\mathbf{r})\right]\phi_{\alpha'}(\mathbf{r})a_{\alpha'} \\ &\quad + \frac{1}{i\hbar}\int d\mathbf{r}\phi^*_\alpha(\mathbf{r})\sum_{\alpha'}\phi_{\alpha'}(\mathbf{r})[a_{\alpha'},\mathbf{H}] \\ &= \frac{1}{i\hbar}\sum_{\alpha'} Z_{\alpha\alpha'}a_{\alpha'} + \frac{1}{i\hbar}[a_\alpha,\mathbf{H}],\end{aligned} \tag{19}$$

with

$$Z_{\alpha\alpha'} = i\hbar\int d\mathbf{r}\left[\frac{d}{dt}\phi^*_\alpha(\mathbf{r})\right]\phi_{\alpha'}(\mathbf{r}). \tag{20}$$

By comparing the above result with the general structure of the Heisenberg equation in Eq. (16), we finally get

$$\frac{d}{dt}a_\alpha\bigg|_{\mathbf{H}} = \frac{1}{i\hbar}[a_\alpha,\mathbf{H}] \tag{21}$$

and

$$\frac{d}{dt}a_\alpha\bigg|_{\phi} = \frac{1}{i\hbar}\sum_{\alpha'} Z_{\alpha\alpha'}a_{\alpha'}. \tag{22}$$

As shown in Ref. 6, the matrix elements $Z_{\alpha\alpha'}$—absent for the case of a time-independent basis—describe the well-known Zener tunneling, i.e., a purely coherent interband dynamics induced by the field.

By combining Eqs. (14) and (16) and considering the explicit form of the total Hamiltonian (1), we get the following equation of motion for ρ:

$$\frac{d}{dt}\rho_{\alpha_1\alpha_2} = \frac{d}{dt}\rho_{\alpha_1\alpha_2}\bigg|_{\mathbf{H}_0} + \frac{d}{dt}\rho_{\alpha_1\alpha_2}\bigg|_{\mathbf{H}_{cp}} + \frac{d}{dt}\rho_{\alpha_1\alpha_2}\bigg|_{\phi}. \tag{23}$$

The first, Liouville-like, term is due to the single-particle Hamiltonian $\mathbf{H}_o$, the second term is due to the carrier-phonon coupling, while the last one is again due to the possible time variation of the basis states α.

More specifically, the time variation due to the free-carrier + free-phonon Hamiltonian $\mathbf{H}_o = \mathbf{H}_c + \mathbf{H}_p$ is given by

$$\frac{d}{dt}\rho_{\alpha_1\alpha_2} = -i\omega_{\alpha_1\alpha_2}\rho_{\alpha_1\alpha_2} \tag{24}$$

with $\omega_{\alpha_1\alpha_2} = (\epsilon_{\alpha_1} - \epsilon_{\alpha_2})/\hbar$.

In a similar way, starting from Eq. (19), the term due to the explicit time variation of our basis set comes out to be of the form

$$\frac{d}{dt}\rho_{\alpha_1\alpha_2}\bigg|_{\phi}=\frac{1}{i\hbar}\sum_{\alpha_1'\alpha_2'}[Z_{\alpha_1\alpha_1'}\delta_{\alpha_2\alpha_2'}-Z^*_{\alpha_2\alpha_2'}\delta_{\alpha_1\alpha_1'}]\rho_{\alpha_1'\alpha_2'}. \tag{25}$$

Compared to the free term in Eq. (24), here we deal with nondiagonal coupling terms.

Let us now come to the carrier-phonon coupling term; its explicit form is obtained using the commutation properties of our creation and destruction operators and may be expressed as

$$\frac{d}{dt}\rho_{\alpha_1\alpha_2}\bigg|_{\mathbf{H}_{cp}}=\sum_{\alpha',\mathbf{q}}\left[\frac{1}{i\hbar}(g_{\alpha_1\alpha',\mathbf{q}}s_{\alpha'\alpha_2,\mathbf{q}}-g_{\alpha'\alpha_2,\mathbf{q}}s_{\alpha_1\alpha',\mathbf{q}})+\text{H.c.}\right], \tag{26}$$

where

$$g_{\alpha\alpha',\mathbf{q}}=\gamma_{\mathbf{q}}\int d\mathbf{r}\phi^*_{\alpha}(\mathbf{r})e^{i\mathbf{q}\cdot\mathbf{r}}\phi_{\alpha'}(\mathbf{r}) \tag{27}$$

denote the matrix elements of the carrier-phonon coupling in Eq. (4) while

$$s_{\alpha\alpha',\mathbf{q}}=\langle a^{\dagger}_{\alpha'}b_{\mathbf{q}}a_{\alpha}\rangle \tag{28}$$

are the so-called phonon-assisted density matrices.[20] These quantities describe many-particle correlations between carriers and phonons.

Equation (23) is thus the starting point of an infinite hierarchy involving higher-order density matrices. To obtain a solution—i.e., a closed set of equations—this hierarchy has to be truncated at some level. As discussed in Ref. 20, in order to properly describe carrier-phonon scattering, the time evolution of the phonon-assisted density matrix $s_{\alpha\alpha',\mathbf{q}}$ should be explicitly considered; its equation of motion has again the structure of Eq. (23), i.e.,

$$\frac{d}{dt}s_{\alpha_1\alpha_2,\mathbf{q}}=-i\Omega^{+}_{\alpha_1\alpha_2,\mathbf{q}}s_{\alpha_1\alpha_2,\mathbf{q}}+y^{cp}_{\alpha_1\alpha_2,\mathbf{q}}+\frac{d}{dt}s_{\alpha_1\alpha_2,\mathbf{q}}\bigg|_{\phi}, \tag{29}$$

with $\Omega^{\pm}_{\alpha_1\alpha_2,\mathbf{q}}=\omega_{\alpha_1\alpha_2}\pm\omega_{\mathbf{q}}$ and

$$\frac{d}{dt}s_{\alpha_1\alpha_2,\mathbf{q}}\bigg|_{\phi}=\frac{1}{i\hbar}\sum_{\alpha_1'\alpha_2'}[Z_{\alpha_1\alpha_1'}\delta_{\alpha_2\alpha_2'}-Z^*_{\alpha_2\alpha_2'}\delta_{\alpha_1\alpha_1'}]s_{\alpha_1'\alpha_2',\mathbf{q}}. \tag{30}$$

As we can see, the contribution due to the possible time variation of our basis states has exactly the same structure of the corresponding term for ρ in Eq. (25); this is due to the fact that, apart from the phononic operator $b^{\dagger}_{\mathbf{q}}$ (which is time independent), the definitions of ρ and s in terms of fermionic operators coincide [see Eqs. (14) and (28)].

The explicit form of the many-body term $y^{cp}_{\alpha_1\alpha_2,\mathbf{q}}$ involves average values of carrier plus phonon operators, typically four fermionic and two bosonic ones. As anticipated, to get a closed set of equations of motion this hierarchy has to be truncated. This is typically realized by applying to the many-body y term in Eq. (29) a mean-field approximation: the average value of carrier plus phonon operators is factorized into products of average values of carrier and phonon operators.[20] In this way Eqs. (23) and (29) reduce to a closed set of equations for the kinetic variables ρ and s. This approximation scheme constitutes the starting point of the well-known carrier quantum kinetics.[20]

To further simplify the description of the problem, a second approximation is usually introduced: the so-called Markov limit. The latter, discussed below, is obtained via an "adiabatic elimination"[20] of the phonon-assisted density matrices s in Eq. (28).

At this point, a few comments are in order. The mean-field approximation previously introduced can be shown to be basis independent; this means that potential deviations from the exact behavior of the electron-phonon system due to the mean-field approximation do not depend on the choice of the basis states $|\alpha\rangle$. This is true also for basis states which describe physically different quantum states, e.g., noninteracting electron-hole pairs versus excitonic states. In contrast, the Markov limit is intrinsically basis dependent. However, basis states which are mutually connected via a gauge transformation [see Eq. (8)] should lead to the very same carrier-phonon dynamics, independent of the choice of the gauge parameter η. As stressed in the introductory part of the paper, this is definitely not the case for the usual treatment of the ICFE, where the Markov limit within the scalar- and vector-potential gauges leads to different results (see the following section). We shall show (see Sec. II D) that such an anomaly is due to the neglect (in performing the Markov limit) of the time variation of our generic basis states [see last term in Eq. (29)].

C. Conventional Markov procedure

As anticipated, the Markov limit consists in an adiabatic elimination of the phonon-assisted density matrices s from the coupled equations of motion in Eqs. (23) and (29).

More specifically, by neglecting the ϕ term in Eq. (30), i.e., the contribution due to the time variation of the basis states α, the final result is

$$s_{\alpha_1\alpha_2,\mathbf{q}}(t)=\mathcal{D}(\Omega_{\alpha_1\alpha_2,\mathbf{q}})y^{cp}_{\alpha_1\alpha_2,\mathbf{q}}(t), \tag{31}$$

with

$$\mathcal{D}(\Omega_{\alpha_1\alpha_2,\mathbf{q}})=\frac{1}{\pi}\int_0^{\infty}dt\,\exp\left[-i\int_0^t\Omega_{\alpha_1\alpha_2,\mathbf{q}}(t')dt'\right]. \tag{32}$$

By inserting the above formal solution for s into the carrier-phonon contribution of Eq. (26), we finally get a closed equation of motion for the single-particle density matrix ρ. In the low-density limit, i.e., $|\rho_{\alpha\alpha'}|\ll 1$, the carrier-phonon contribution to the dynamics is of the form

$$\left.\frac{d}{dt}\rho_{\alpha_1\alpha_2}\right|_{\mathbf{H}_{cp}} = \sum_{\alpha_1'\alpha_2'} (\Gamma^{\rm in}_{\alpha_1\alpha_2,\alpha_1'\alpha_2'}\rho_{\alpha_1'\alpha_2'} - \Gamma^{\rm out}_{\alpha_1\alpha_2,\alpha_1'\alpha_2'}\rho_{\alpha_1'\alpha_2'}) + \text{H.c.}, \tag{33}$$

where

$$\Gamma^{\rm in}_{\alpha_1\alpha_2,\alpha_1'\alpha_2'} = \frac{\pi}{\hbar^2}\sum_{\pm,\mathbf{q}} \mathcal{N}^{\pm}_{\mathbf{q}} g_{\alpha_1\alpha_1',\mathbf{q}} g^*_{\alpha_2\alpha_2',\mathbf{q}} \mathcal{D}^*(\Omega^{\mp}_{\alpha_2\alpha_2',\mathbf{q}})$$

$$\Gamma^{\rm out}_{\alpha_1\alpha_2,\alpha_1'\alpha_2'} = \frac{\pi}{\hbar^2}\sum_{\pm,\mathbf{q}} \mathcal{N}^{\pm}_{\mathbf{q}} \sum_{\alpha''} g^*_{\alpha''\alpha_1,\mathbf{q}} g_{\alpha''\alpha_1',\mathbf{q}} \mathcal{D}(\Omega^{\pm}_{\alpha''\alpha_1',\mathbf{q}}) \times \delta_{\alpha_2\alpha_2'} \tag{34}$$

are generalized in- and out-scattering rates.[20] Here, the $\pm$ sign refers to phonon emission and absorption, respectively, and $\mathcal{N}^{\pm}_{\mathbf{q}} = N_{\mathbf{q}} + \frac{1}{2} \pm \frac{1}{2}$ denote the corresponding phonon occupation factors.

Equation (33) is the quantum-mechanical generalization of the well-known Boltzmann transport equation;[14] indeed, by neglecting all nondiagonal terms of the single-particle density matrix ($\rho_{\alpha_1\alpha_2} = f_{\alpha_1}\delta_{\alpha_1\alpha_2}$), the latter is easily recovered:

$$\left.\frac{d}{dt}f_\alpha\right|_{\mathbf{H}_{cp}} = \sum_{\alpha'} (P_{\alpha\alpha'}f_{\alpha'} - P_{\alpha'\alpha}f_\alpha). \tag{35}$$

Here, as usual, the scattering rates for in- and out-scattering processes coincide; they correspond to twice the diagonal parts ($\alpha_1\alpha_1' = \alpha_2\alpha_2'$) of the scattering operators $\Gamma^{\rm in}$ and $\Gamma^{\rm out}$ in Eq. (34):[22]

$$P_{\alpha\alpha'} = \frac{2\pi}{\hbar^2}\sum_{\pm,\mathbf{q}} |g_{\alpha\alpha',\mathbf{q}}|^2 \mathcal{N}^{\pm}_{\mathbf{q}} \mathrm{Re}[\mathcal{D}(\Omega^{\pm}_{\alpha\alpha',\mathbf{q}})]. \tag{36}$$

The generalized carrier-phonon scattering rates in Eq. (34)—as well as their semiclassical counterparts in Eq. (36)—involve the $\mathcal{D}$ function in Eq. (32). For the case of a time-independent basis set, i.e., $\eta = 0$ (Wannier-Stark states), the detuning frequency Ω is also time independent and the real part of the function $\mathcal{D}$ in Eq. (32) gives the well-known energy-conserving Dirac δ function and Eq. (36) is exactly the usual Fermi's golden rule; in contrast, for the case of a time dependent basis, i.e., $\eta = 1$ (accelerated Bloch states), the detuning is time dependent, leading to a broader function $\mathcal{D}$.[10] This is exactly the ICFE previously introduced:[9] due to the field-induced variation of the carrier wave vector $\mathbf{k}$, the energy difference between initial and final states ($\epsilon_{\mathbf{k}(t)} - \epsilon_{\mathbf{k}(t)\pm\mathbf{q}}$) changes in time giving rise to multiple and/or broad resonances in the carrier-phonon scattering process. Such energy-nonconserving scenario has no counterpart in the Wannier-Stark picture.[23] This clearly shows that the generalized scattering rates in Eq. (34) are not gauge invariant.

D. Gauge-invariant formulation

The aim of this paper is to show that the derivation recalled so far is only valid within the Wannier-Stark picture ($\eta = 0$). Indeed, as anticipated, the crucial point is the neglect of the possible time variation of our basis states α.

More specifically, a proper inclusion of the ϕ terms in Eq. (30) suggests to rewrite Eq. (29) as

$$\frac{d}{dt}s_{\alpha_1\alpha_2,\mathbf{q}} = -i\sum_{\alpha_1'\alpha_2'} \tilde{\Omega}^{+}_{\alpha_1\alpha_2,\alpha_1'\alpha_2',\mathbf{q}} s_{\alpha_1'\alpha_2',\mathbf{q}} + y^{cp}_{\alpha_1\alpha_2,\mathbf{q}} \tag{37}$$

with

$$\hbar\tilde{\Omega}^{\pm}_{\alpha_1\alpha_2,\alpha_1'\alpha_2',\mathbf{q}} = \mathcal{E}_{\alpha_1\alpha_1'}\delta_{\alpha_2\alpha_2'} - \mathcal{E}^*_{\alpha_2\alpha_2'}\delta_{\alpha_1\alpha_1'} \pm \hbar\omega_{\mathbf{q}}\delta_{\alpha_1\alpha_2,\alpha_1'\alpha_2'} \tag{38}$$

and

$$\mathcal{E}_{\alpha\alpha'} = \epsilon_\alpha\delta_{\alpha\alpha'} + Z_{\alpha\alpha'}. \tag{39}$$

It is possible to show that $\mathcal{E}_{\alpha\alpha'}$ correspond to the matrix elements of the single-particle Hamiltonian (9) for $\eta = 0$, i.e., written in the scalar-potential gauge. This can be easily verified for the two particular choices of our basis set α, the scalar- and the vector-potential ones. It follows that *for a generic time-dependent basis, Eq. (37) has a nondiagonal structure*, and therefore *it does not allow a simple exponential solution*. This implies that for $\eta \neq 0$ the Markov limit is not straightforward.

The correct procedure—i.e., gauge invariant—is (i) *to perform a unitary transformation which diagonalizes the superoperator* $\tilde{\Omega}$ in Eq. (38), and (ii) *to perform the exponential formal integration described above*. Since $\mathcal{E}_{\alpha\alpha'}$ are the matrix elements of $\mathbf{H}_c$ for $\eta = 0$ (scalar-potential gauge), the unitary transformation that diagonalizes $\tilde{\Omega}$ is just $\mathcal{U}^{0,\eta}$, i.e., the transformation connecting the generic gauge η to the scalar-potential basis ($\eta = 0$). We stress that the new diagonal elements coincide with the eigenvalues of $\tilde{\Omega}$ which, in turn, correspond to the *time-independent detuning functions* $\Omega_{\alpha_1\alpha_2,\mathbf{q}}$ *in the Wannier-Stark gauge*.

This clearly shows that the Markov limit used to derive the generalized Boltzmann equation in Eq. (33) is only well defined in the Wannier-Stark picture, for which the various ϕ terms vanish and the detuning functions Ω are time independent.

This does not violate the gauge-invariant nature of our formulation. Indeed, given the generalized Boltzmann equation (33) written in the scalar-potential picture, the latter can be written in any generic gauge η by applying the unitary transformation $\mathcal{U}$ introduced in Eq. (13). To this end, let us introduce the single-particle density-matrix operator

$$\rho = \sum_{\alpha_1\alpha_2} |\alpha_1\rangle\rho_{\alpha_1\alpha_2}\langle\alpha_2|, \tag{40}$$

which is by definition gauge invariant/η-independent. This suggests to write the generalized Boltzmann equation (33) in an operatorial form as

$$\left.\frac{d}{dt}\rho\right|_{\mathbf{H}_{cp}} = (\Gamma^{\rm in}\rho - \Gamma^{\rm out}\rho) + \text{H.c.}, \tag{41}$$

where

$$\Gamma^{\text{in/out}}=\sum_{\alpha_1\alpha_2,\alpha_1'\alpha_2'}|\alpha_1\rangle|\alpha_1'\rangle\Gamma^{\text{in/out}}_{\alpha_1\alpha_2,\alpha_1'\alpha_2'}\langle\alpha_2|\langle\alpha_2'| \quad (42)$$

are in- and out-scattering superoperators.

As already stressed, our aim is to propose a gauge-invariant formulation of the problem. This requires the superoperators in Eq. (42) to be η independent as well. The analysis presented so far has shown that the scattering matrices $\Gamma^{\text{in/out}}_{\alpha_1\alpha_2,\alpha_1'\alpha_2'}$ are only well defined in the Wannier-Stark picture ($\eta=0$). They are no longer probabilities and exhibit a superoperator structure; for this reason their gauge-invariant extension to any generic η value is realized by the following four-index unitary transformation:

$$\Gamma^{\eta}_{\alpha_1\alpha_2,\alpha_1'\alpha_2'}=U_{\bar{\alpha}_1\bar{\alpha}_3}U_{\bar{\alpha}_1'\bar{\alpha}_3'}\Gamma^{\bar{\eta}=0}_{\bar{\alpha}_3\bar{\alpha}_4,\bar{\alpha}_3'\bar{\alpha}_4'}U_{\bar{\alpha}_4\bar{\alpha}_2}U_{\bar{\alpha}_4'\bar{\alpha}_2'} \quad (43)$$

(implicit summation over repeated indices is assumed), where $U_{\bar{\alpha}\bar{\alpha}'}$ are the matrix elements of the unitary transformation $\mathcal{U}^{0,\eta}$ in the Wannier-Stark picture ($\bar{\eta}=0$).

Equation (43) is the gauge-invariant formulation of Fermi's golden rule we were looking for. Contrary to the conventional approach, in the case of a time-dependent basis, e.g., accelerated Bloch states,[4] instead of using Eq. (34) with an *ad hoc* energy-nonconserving $\mathcal{D}$ function, the correct procedure is to compute the generalized scattering rates (34) in the Wannier-Stark picture, and then to apply the gauge transformation $\mathcal{U}_{\eta,0}$ according to Eq. (43). Thus the desired gauge-invariant equation of motion (i.e., valid for any η) turns out to be again Eq. (33), where the scattering operators Γ need to be replaced by their gauge-invariant version Γ^{η}.

III. A FEW SIMULATED EXPERIMENTS

In order to quantitatively assess the magnitude and physical implications of the wrong estimation of carrier-phonon scattering within the usual treatment of the ICFE previously discussed, we have performed fully three-dimensional (3D) calculations of high-field charge transport in state-of-the-art semiconductor nanostructures. In particular, aim of our 3D description was to properly treat—in addition to the carrier quantum confinement along the growth direction—the in-plane energy relaxation and thermalization dynamics.

As recalled in the introductory part of the paper, any single-particle quantity A—e.g., charge current, carrier drift velocity, mean kinetic energy, etc.—may be evaluated starting from the single-particle density matrix in Eq. (14) according to

$$\langle A\rangle=\text{tr}\{\mathbf{A}\rho\}=\sum_{\alpha_1\alpha_2}A_{\alpha_1\alpha_2}\rho_{\alpha_2\alpha_1}, \quad (44)$$

where $\mathbf{A}$ is the single-particle operator describing the physical quantity A and $A_{\alpha_1\alpha_2}=\langle\alpha_1|\mathbf{A}|\alpha_2\rangle$ are its matrix elements within the gauge-dependent representation α. The quantity in Eq. (44) describes a physical property of the system and, as such, should be gauge invariant; indeed, this can be easily verified recalling that the density-matrix operator in Eq. (40) is itself η independent. It follows that, in order to evaluate the trace in Eq. (44), one may chose the value of the gauge parameter η in the most convenient way. According to the analysis presented in Sec. II D, the only basis in which the Markov limit is properly defined is the Wannier-Stark one. This suggests to evaluate the density matrix $\rho_{\alpha_1\alpha_2}$ directly in this time-independent representation ($\eta=0$).

Since our primary goal is to investigate high-field transport in steady-state conditions, we focus on the stationary solution of the quantum-transport equation in Eq. (23), i.e.,

$$\frac{d}{dt}\rho_{\alpha_1\alpha_2}=\frac{d}{dt}\rho_{\alpha_1\alpha_2}\bigg|_{\mathbf{H}_0}+\frac{d}{dt}\rho_{\alpha_1\alpha_2}\bigg|_{\mathbf{H}_{cp}}+\frac{d}{dt}\rho_{\alpha_1\alpha_2}\bigg|_{\phi}=0. \quad (45)$$

By combining the free-carrier term in Eq. (24) with the generalized scattering dynamics in Eq. (33), and recalling that for $\eta=0$ all the ϕ terms vanish, we get the following steady-state equation for $\rho_{\alpha_1\alpha_2}$ in the Wannier-Stark picture:

$$\frac{d}{dt}\rho_{\alpha_1\alpha_2}=\sum_{\alpha_1'\alpha_2'}\mathcal{L}_{\alpha_1\alpha_2,\alpha_1'\alpha_2'}\rho_{\alpha_1'\alpha_2'}=0, \quad (46)$$

where

$$\mathcal{L}_{\alpha_1\alpha_2,\alpha_1'\alpha_2'}=-i\omega_{\alpha_1\alpha_2}\delta_{\alpha_1\alpha_2,\alpha_1'\alpha_2'}+\Gamma^{\text{in}}_{\alpha_1\alpha_2,\alpha_1'\alpha_2'}-\Gamma^{\text{out}}_{\alpha_1\alpha_2,\alpha_1'\alpha_2'} \quad (47)$$

can be regarded as an effective Liouville superoperator acting on our single-particle density matrix. By introducing the compact notation $i\equiv\alpha_1\alpha_2$, the above steady-state equation can be rewritten as

$$\mathcal{L}_{ii'}\rho_{i'}=0. \quad (48)$$

As usual, the nontrivial solutions—i.e., different from zero—of this homogeneous linear problem correspond to the singular solutions of the Liouville superoperator (47), i.e., to the $\lambda=0$ solution of the eigenvalue problem

$$\mathcal{L}_{ii'}\rho_{i'}=\lambda\rho_i. \quad (49)$$

Our numerical approach is then based on a direct diagonalization of the Liouville superoperator $\mathcal{L}$ in Eq. (47). The steady-state density matrix ρ we are looking for will thus correspond to the $\lambda=0$ eigenvector $\rho_i\equiv\rho_{\alpha_1\alpha_2}$.

In the absence of carrier-phonon scattering it is easy to verify that any diagonal density matrix $\rho_{\alpha_1\alpha_2}=f_{\alpha_1}\delta_{\alpha_1\alpha_2}$ is a possible solution of the steady-state transport equation in Eq. (46). This amounts to saying that in this case the eigenvalue spectrum contains the $\lambda=0$ value only. Indeed, physically speaking, in the phonon-free case any initial "semiclassical state"—corresponding to a given population f_α of the Wannier-Stark states without any interlevel phase coherence—will not be altered by the free-carrier system Hamiltonian [see Eq. (24)].

In contrast, in the presence of carrier-phonon interaction the eigenvalue spectrum of the Liouville superoperator $\mathcal{L}$ exhibits a single (i.e., nondegenerate) $\lambda=0$ eigenvalue, and

therefore a unique stationary solution $\rho_{\alpha_1\alpha_2}$. Moreover, in the presence of carrier-phonon coupling the Liouville superoperator $\mathcal{L}$ contains nondiagonal elements: $\mathcal{L}_{\alpha_1\alpha_2\neq\alpha_1'\alpha_2'}$. This, in turn, may give rise to a nondiagonal steady-state density matrix, which may be regarded as a residual single-particle phase coherence.

Given the stationary single-particle density matrix $\rho_{\alpha_1\alpha_2}$, we finally compute any physical quantity of interest according to Eq. (44). To this end, the only ingredients needed are the matrix elements $A_{\alpha_1\alpha_2}$ of the physical quantity under investigation [see Eq. (44)].

In order to better evaluate the results of the gauge-invariant calculation described so far, we have also implemented a corresponding calculation based on the semiclassical treatment of the ICFE within the vector-potential picture described in Sec. II C. In this case, by combining the explicit form of the ϕ terms in Eq. (25) with the "*ad hoc*" Boltzmann-like collision operator in Eq. (35) and neglecting interband ($\nu\rightarrow\nu'$) Zener tunneling, the steady-state transport equation (45) reduces to a semiclassical equation of the form

$$-e\frac{\mathbf{F}}{\hbar}\cdot\nabla_{\mathbf{k}}f_{\mathbf{k}\nu}+\sum_{\mathbf{k}'\nu'}(P_{\mathbf{k}\nu,\mathbf{k}'\nu'}f_{\mathbf{k}'\nu'}-P_{\mathbf{k}'\nu',\mathbf{k}\nu}f_{\mathbf{k}\nu})=0. \tag{50}$$

Here, the first contribution is the well-known drift term—describing the intraband carrier acceleration induced by the applied field $\mathbf{F}$—while the explicit form of the scattering rates P are given in Eq. (36) written in the vector-potential gauge: $\alpha=\mathbf{k}(t),\nu$. As for the gauge-invariant calculation previously described, also in this case we deal with a homogeneous linear transport equation for $f_{\mathbf{k}\nu}$. By introducing a suitable $\mathbf{k}$-space discretization, the steady-state transport equation in Eq. (50) can be easily transformed into a corresponding eigenvalue problem, whose $\lambda=0$ solution provides the desired steady-state carrier distribution. Given such steady-state solution $f_{\mathbf{k}\nu}$, we may obtain any generic single-particle physical quantity via the semiclassical version of Eq. (44), i.e.,

$$\langle A\rangle=\sum_{\mathbf{k}\nu}A_{\mathbf{k}\nu,\mathbf{k}\nu}f_{\mathbf{k}\nu}. \tag{51}$$

Finally, in order to compare the two ICFE treatments discussed so far with the genuine Boltzmann theory—where the ICFE is simply neglected—we shall replace the "*ad hoc*" scattering rates P in Eq. (36) with the standard rates given by Fermi's golden rule, i.e.,

$$P^{o}_{\alpha\alpha'}=\frac{2\pi}{\hbar^2}\sum_{\pm,\mathbf{q}}|g_{\alpha\alpha',\mathbf{q}}|^2\mathcal{N}^{\pm}_{\mathbf{q}}\delta(\Omega^{\pm}_{\alpha\alpha',\mathbf{q}}). \tag{52}$$

As prototypical system, we have considered a state-of-the-art GaAs-based nanometric superlattice. More specifically, we have performed a detailed investigation of the 45 Å/45 Å GaAs/$Al_{0.3}Ga_{0.7}As$ superlattice structure shown in Fig. 1. The single-particle carrier states $\{|\alpha\rangle\}$ are described

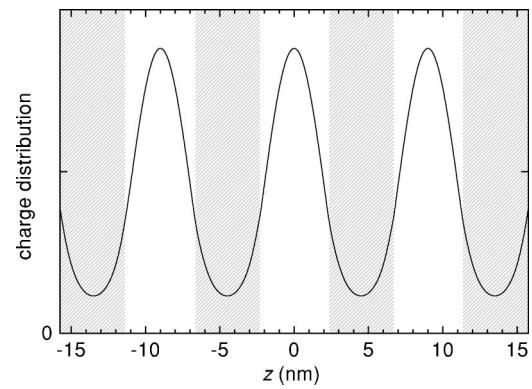

FIG. 1. Schematics of the prototypical 45 Å/45 Å GaAs/$Al_{0.3}Ga_{0.7}As$ superlattice structure considered in our simulated experiments: Real-space periodic nanostructure profile (shaded regions correspond to barriers) and charge distribution corresponding to the ground-state ($k_\parallel=0$) envelope function in the field-free case ($n(r_\parallel)\propto|\phi^{o}_{k_\parallel=0,\nu=1}(r_\parallel)|^2$) (see text).

withinthe usual envelope-function approximation in terms of a space-independent effective mass m^*. They come out to be products of two-dimensional plane waves and one-dimensional envelope functions:

$$\phi_\alpha(\mathbf{r})=\frac{1}{\sqrt{\Omega}}e^{i\mathbf{k}_\perp\cdot\mathbf{r}_\perp}\phi^{\parallel}_{\alpha_\parallel}(r_\parallel), \tag{53}$$

Ω denoting a suitable normalization area.

In the free-field case, the envelope functions $\phi^{\parallel}$ in Eq. (53) reduce to one-dimensional Bloch states $\phi^{\parallel}_{k_\parallel\nu}$ corresponding to the periodic heterostructure potential reported in the inset of Fig. 2. As we can see, we deal with a relatively small band-edge discontinuity ($V_o=250$ meV). The latter, combined with a barrier width of 45 Å, gives rise to significant interwell carrier tunneling. This is confirmed by the field-free ground-state charge distribution (solid curve in Fig. 1), which shows a clear fingerprint of carrier delocalization.

The interwell coupling displayed in Fig. 1 should translate into a dispersive energy-momentum relation along the growth direction. This is confirmed by the superlattice mini-

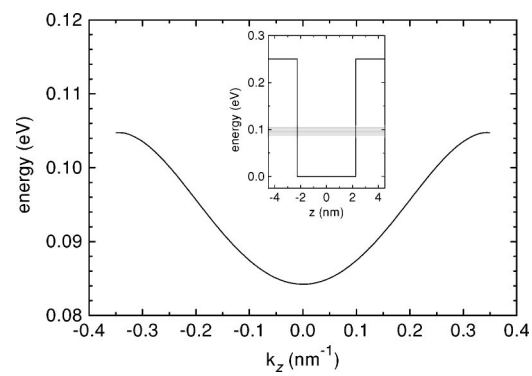

FIG. 2. Single-miniband diagram (miniband width of about 20 meV) corresponding to the superlattice structure depicted in Fig. 1. The superlattice potential profile (band-edge discontinuity of 0.25 eV) is also shown in the inset (see text).

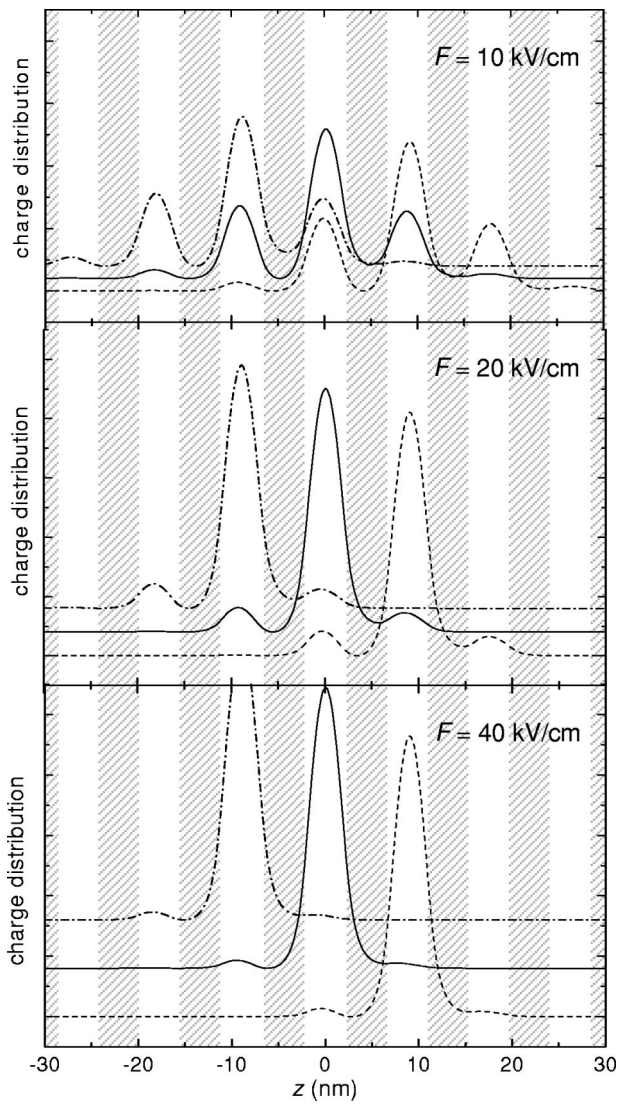

FIG. 3. Charge distribution corresponding to the Wannier-Stark states in the superlattice structure of Fig. 1 for different values of the applied field F. For each field three states are displayed: $n=-1$ (dash-dotted curve), $n=0$ (solid curve), and $n=1$ (dotted curve) (see text).

band profile reported in Fig. 2. As we can see, we deal with a carrier miniband only; the latter has a width of about 20 meV, which is smaller than the LO-phonon energy. For this reason, generally speaking, carrier-LO phonon scattering (in particular, emission processes) is accompanied by a significant perpendicular (in-plane) versus parallel energy transfer (see below).

In the presence of an applied field F along the growth direction, the one-dimensional envelope functions $\phi^{\parallel}$ within the scalar-potential gauge ($\eta=0$) correspond to the usual Wannier-Stark states. The latter are displayed in Fig. 3 for different values of the applied field. As we can see, for increasing values of the field we deal with an increasing state localization and a corresponding suppression of interwell single-particle tunneling.

The primary goal of our simulated experiments was the study of the current-voltage characteristics of the superlattice

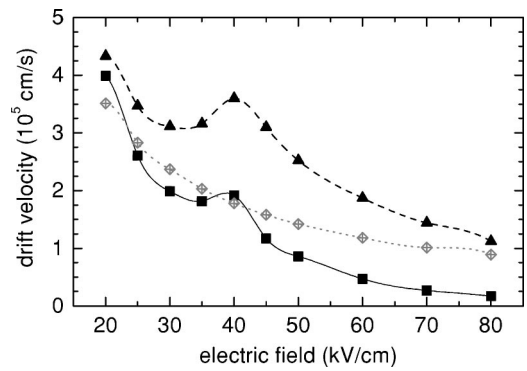

FIG. 4. Steady-state carrier drift velocity as a function of the applied field for the superlattice structure of Fig. 1 at room temperature in the low-density limit. Gauge-invariant result (squares), conventional ICFE model (triangles), and Boltzmann limit (diamonds) (see text). Lines are a guide to the eye.

structure previously introduced in the presence of carrier-LO phonon scattering. More specifically, we have evaluated the carrier drift velocity as a function of the applied field. The latter can be readily computed according to Eq. (44), using as single-particle quantity the velocity operator:

$$\mathbf{A}=\frac{\mathbf{P}}{m^*}=-\frac{i\hbar}{m^*}\boldsymbol{\nabla}. \tag{54}$$

Figure 4 shows the steady-state carrier drift velocity as a function of the applied field for the superlattice structure of Fig. 1 at room temperature in the low-density limit. Here, we compare the usual ICFE model [see Eq. (50)] (triangles) to the result of the proposed gauge-invariant approach [see Eqs. (41), (43), and (46)] (squares). At low fields the two curves exhibit a similar behavior, but they tend to separate as the field increases. In particular, the drift velocity corresponding to the usual ICFE treatment within the accelerated-Bloch-state picture at high fields is by far higher than the gauge-invariant one; this is exactly the potential overestimation of the ICFE previously identified: due to the neglect of the non-diagonal Zener-like terms in Eq. (37)—induced by the time variation of the basis states—one underestimates the carrier-phonon coupling, thus leading to significant overestimations of carrier drift velocity and current. The peak at $\sim$40 kV/cm, in both curves, corresponds to the phonon resonance, i.e., for this value of the applied field F the Wannier-Stark or Bloch energy eFd is equal to the LO-phonon energy.

Let us finally compare the two quantum-mechanical results (squares and triangles) with the purely semiclassical (Boltzmann) one [see Eqs. (50) and (52)] (diamonds). The latter shows a good agreement with the gauge-invariant one (squares) for a wide field range (20–50 kV/cm), while it differs significantly from the standard ICFE model (triangles).

As anticipated, this may partially account for the surprisingly good agreement between semiclassical and rigorous

quantum-transport calculations reported in Refs. 10 and 12, as well as for the anomalous carrier heating typical of standard ICFE models.[15]

We stress that the numerical analysis presented so far, based on a superlattice structure, may differ quantitatively from the case of a bulk semiconductor. The main reason is that the superlattice miniband width in Fig. 2 is smaller than the phonon energy; it follows that an electron with zero or negligible in-plane momentum is not able to reach the phonon-emission threshold. However, in the presence of a strong applied field, the carriers will experience a strong parallel-to-perpendicular energy transfer; it follows that in the high-field regime of Fig. 4 the average electron energy is typically much higher than the phonon energy, thus allowing for carrier-phonon scattering. We can thus conclude that in bulk systems the current overestimation previously identified could be of smaller magnitude, but qualitatively speaking we expect a similar behavior.

As final remark, we stress that the choice of Wannier-Stark basis states used to evaluate the current-voltage characteristics becomes problematic in the low-field regime ($F \to 0$) as well as in the bulk limit ($d \to a$). Indeed in both cases the Wannier-Stark energy $\Delta\epsilon = eFd$ is much smaller than the phonon energy; this requires to include in our simulation a relatively high number of Wanier-Stark states. However, apart from this purely technical limitation, there is no principle problem to apply the approach presented so far to bulk systems.

IV. SUMMARY AND CONCLUSIONS

In summary, we have revisited the standard treatment of carrier-phonon scattering in the presence of high electric fields by means of a gauge-invariant density-matrix formalism. The proposed formulation of the quantum-transport problem has allowed us, on the one hand, to derive a gauge-independent formulation of Fermi's golden rule; on the other hand, our analysis has clearly shown that the conventional description of high-field carrier-phonon scattering does not account for the possible variation of our single-particle basis states. This is recognized to be the origin of the apparent discrepancy between scalar- and vector-potential treatments of the problem; indeed, a proper account of such contributions leads, in general, to an ill-defined Markov limit in the carrier-phonon interaction process, attributing to the scalar-potential or Wannier-Stark picture a privileged role. Starting from the generalized scattering rates evaluated within the scalar-potential picture, we have extended their definition to any generic gauge η via a corresponding unitary transformation within our single-particle state space.

The neglect of such Zener-like contributions in the transport equation is shown to lead to a wrong estimation of the high-field voltage-current characteristics, and may partially account for the surprisingly good agreement between semiclassical and rigorous quantum-transport calculations previously reported. This has been confirmed by fully three-dimensional simulations of charge transport in state-of-the-art semiconductor superlattices, which show a significant current overestimation.

From our analysis we can conclude that, in addition to the Markov approximation, the neglect of nondiagonal density-matrix elements—typical of the standard Boltzmann transport theory—may lead to nonphysical results; indeed, the latter, being intrinsically basis dependent, is not compatible with the gauge-invariant formulation of the problem.

We finally stress that the above conclusions are not peculiar of the carrier-phonon coupling considered in the paper; in contrast, they apply to any single-particle interaction mechanism, such carrier-plasmon and carrier-impurity scattering, and in principle can be extended to two-body interactions, such as carrier-carrier scattering.

*Electronic mail: Emanuele. Ciancio@PoliTo.It
†Electronic mail: Rita. Iotti@INFM. PoliTo.It
‡Electronic mail: Fausto. Rossi@PoliTo.It

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[15] See, e. g., L. Reggiani, P. Lugli, and A.P. Jauho, Phys. Rev. B **36**, 6602 (1987), and references therein.
[16] The need for a gauge-invariant formulation of the problem was originally pointed out by Bertoncini and Jauho in Ref. 11.
[17] Indeed, it is easy to verify that for any value of η—corresponding to a different Hamiltonian $\mathbf{H}_c$ in Eq. (9)—we are describing exactly the same electric field $\mathbf{F}$:

$$\mathbf{F}_\eta(\mathbf{r},t) = -\nabla\varphi_\eta(\mathbf{r}) - \frac{1}{c}\frac{\partial}{\partial t}\mathbf{A}_\eta(t) = \mathbf{F},$$

$$\mathbf{B}_\eta(\mathbf{r},t) = \nabla\times\mathbf{A}_\eta(t) = 0. \qquad (55)$$

[18] We stress that this is not the more general gauge choice, indeed it hides some definite conditions. We do not want to discuss the general electromagnetic problem here; indeed, we consider a very specific case: a static homogeneous electric field with no magnetic field.

[19] Contrary to the conventional time-dependent perturbation theory, we thus propose a kinetic description based on a time-dependent quantum-mechanical representation.

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[21] This is defined as the average value of two creation and destruction operators: its diagonal elements $f_\alpha = \rho_{\alpha\alpha}$ correspond to the usual distribution functions of the semiclassical Boltzmann theory while the off-diagonal terms $(\alpha_1 \neq \alpha_2)$ describe the degree of quantum-mechanical phase coherence between states α_1 and α_2.

[22] Such semiclassical rates exhibit the well-known structure of Fermi's golden rule; they describe the scattering probability for a phonon-induced transition between states α and α'. Their quantum-mechanical—or nondiagonal—generalization is then given by the scattering matrices $\Gamma^{\text{in/out}}$, which describe the effect on the time evolution of the density-matrix element $\rho_{\alpha_1\alpha_2}$ due to the generic element $\rho_{\alpha_1'\alpha_2'}$.

[23] The presence of other interaction mechanisms, such as carrier-carrier and carrier-plasmon scattering, may give rise to additional "intracollisional effects;" in this case the main feature is a single-particle spectral broadening usually referred to as "collisional broadening" (Ref. 20). Such an effect can be easily included in our theoretical approach by adding an imaginary contribution to the self-energy Ω in Eq. (32). However, in the low-density limit considered in our simulated experiments such collisional-broadening effects are expected to be negligible.