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Microscopic modeling of scattering quantum non-locality in semiconductor nanostructures

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In spite of their intrinsic validity limits, a number of Boltzmann-like simulation schemes are extensively employed in the investigation of semiconductor nanomaterials and nanodevices. Such modeling strategies, based on the neglect of carrier phase coherence, are definitely unable to describe space-dependent ultrafast phenomena. In this letter, we shall propose a quantum-mechanical modeling strategy able to properly account for scattering-induced spatial non-locality. Its power and flexibility will be demonstrated via a few simulated experiments. © *2013 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4821158]

Following the path paved by the early proposal by Esaki and Tsu,[1] artificially tailored as well as self-assembled semiconducting heterostructures at the nanoscale now form the leading edge of semiconductor science and technology.[2–4] The design of modern optoelectronic devices, in fact, heavily exploits the principles of band-gap engineering,[5] achieved by confining charge carriers in spatial regions comparable to their de Broglie wavelengths. This, together with the progressive reduction of the typical time-scales involved, pushes device miniaturization toward limits where the application of the traditional Boltzmann transport theory[6] becomes questionable, and a comparison with more rigorous quantum-transport approaches[7–13] is imperative. However, in spite of the quantum-mechanical nature of electron and photon dynamics in the core region of typical solid-state nanodevices (e.g., quantum dots[14,15] and graphene-based structures[16,17]) the overall behavior of such quantum systems is often governed by a highly non-trivial interplay between phase coherence and dissipation/dephasing.[10,11]

In spite of the intrinsic validity limits just recalled, during the last decades, a number of Boltzmann-like Monte Carlo simulation schemes have been extensively employed for the investigation of new-generation semiconductor nanodevices.[18–27] Such modeling strategies—based on the neglect of carrier phase coherence (see below)—are however unable to properly describe space-dependent ultrafast phenomena. To this aim, the crucial step is to adopt a quantum-mechanical description of the carrier subsystem; this can be performed at different levels, ranging from phenomenological dissipation/decoherence models[5] to quantum-kinetic treatments.[10,11] Indeed, in order to overcome the intrinsic limitations of the semiclassical picture in properly describing ultrafast space-dependent phenomena—e.g., real-space transfer and escape versus capture processes—Jacoboni and co-workers have proposed a quantum Monte Carlo technique,[28] while Kuhn and co-workers have proposed a quantum-kinetic treatment;[29] however, due to their high computational cost, these non-Markovian density-matrix approaches are currently unsuitable for the design and optimization of new-generation nanodevices.

Aim of this letter is to propose a conceptually and computationally simple as well as physically reliable quantum-mechanical generalization of the conventional Boltzmann theory, able to preserve the power and flexibility of the semiclassical picture in describing a large variety of scattering mechanisms; more specifically, employing a microscopic derivation of generalized scattering rates based on a recent reformulation of the Markov limit,[30] we shall propose a density-matrix equation able to properly account for space-dependent ultrafast dynamics, and in particular to study scattering-induced non-locality effects.

The crucial interplay between phase coherence and dissipation/decoherence phenomena may be conveniently described through the equation of motion for the electronic single-particle density matrix[10,13]

$$\frac{d\rho_{\alpha_1\alpha_2}}{dt} = \left.\frac{d\rho_{\alpha_1\alpha_2}}{dt}\right|_{\rm sp} + \left.\frac{d\rho_{\alpha_1\alpha_2}}{dt}\right|_{\rm mb}, \tag{1}$$

where

$$\left.\frac{d\rho_{\alpha_1\alpha_2}}{dt}\right|_{\rm sp} = \frac{\epsilon_{\alpha_1} - \epsilon_{\alpha_2}}{i\hbar}\rho_{\alpha_1\alpha_2} \tag{2}$$

accounts for the coherent evolution dictated by the non-interacting single-particle Hamiltonian (here, α and ϵ_α denote the single-particle eigenstates and energy levels corresponding to the nanodevice potential profile), while the last (many-body) term encodes dissipation and decoherence processes, arising from the energy exchange between the carriers and the host material. Equation (1) applies to a broad variety of problems ranging from quantum-transport to ultrafast-optics phenomena, a remarkable example being the semiconductor Bloch equations.[10]

It is crucial to stress that the degree of accuracy of the density-matrix equation (1) is intimately related to an appropriate choice of its last term. Indeed, oversimplified phenomenological treatments can lead, for instance, to a violation of the positive-definite character of the density matrix $\rho_{\alpha_1\alpha_2}$, a

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mandatory prerequisite of any quantum-mechanical time evolution fulfilled, e.g., by employing a so-called Lindblad superoperator.[31] To overcome this serious limitation, an alternative Markov procedure has recently been proposed.[30] Following this alternative adiabatic-decoupling scheme, it is possible to perform a microscopic derivation of a Lindblad-like scattering superoperator; more specifically, for any one-electron interaction mechanism s (carrier-phonon, carrier-plasmon, carrier-impurity scattering, etc.) in the low-density limit one gets

$$\left.\frac{d\rho_{\alpha_1\alpha_2}}{dt}\right|_{\rm mb} = \frac{1}{2}\sum_s \sum_{\alpha_1'\alpha_2'} \left[\mathcal{P}^s_{\alpha_1\alpha_2,\alpha_1'\alpha_2'}\rho_{\alpha_1'\alpha_2'} - \mathcal{P}^{s*}_{\alpha_1'\alpha_1',\alpha_1\alpha_2'}\rho_{\alpha_2'\alpha_2}\right] + \text{H.c.} \tag{3}$$

(H.c. denoting the Hermitian conjugate) in terms of generalized scattering rates

$$\mathcal{P}^s_{\alpha_1\alpha_2,\alpha_1'\alpha_2'} = A^s_{\alpha_1\alpha_1'}A^{s*}_{\alpha_2\alpha_2'}, \tag{4}$$

where the explicit form of the Lindblad matrix elements $A^s_{\alpha\alpha'}$ depends on the particular interaction mechanism considered.

The proposed quantum-mechanical generalization is then given by the density-matrix equation (1) equipped with the microscopic scattering superoperator in Eq. (3).

In order to investigate the space dependence of the phenomenon under examination, let us recall the link between our density matrix $\rho_{\alpha_1\alpha_2}$ and the corresponding spatial carrier density, namely,

$$n(\mathbf{r}) = \sum_{\alpha_1\alpha_2} \phi_{\alpha_1}(\mathbf{r})\rho_{\alpha_1\alpha_2}\phi^*_{\alpha_2}(\mathbf{r}), \tag{5}$$

where $\phi_\alpha(\mathbf{r}) = \langle \mathbf{r}|\alpha\rangle$ denotes the real-space wavefunction corresponding to the eigenstate α. Combining the above prescription with the density-matrix equation (1), the time evolution of the spatial carrier density is

$$\frac{\partial n(\mathbf{r})}{\partial t} = \left.\frac{\partial n(\mathbf{r})}{\partial t}\right|_{\rm sp} + \left.\frac{\partial n(\mathbf{r})}{\partial t}\right|_{\rm mb}, \tag{6}$$

with

$$\left.\frac{\partial n(\mathbf{r})}{\partial t}\right|_{\rm sp} = \sum_{\alpha_1\alpha_2} \phi_{\alpha_1}(\mathbf{r})\frac{\epsilon_{\alpha_1}-\epsilon_{\alpha_2}}{i\hbar}\rho_{\alpha_1\alpha_2}\phi^*_{\alpha_2}(\mathbf{r}) \tag{7}$$

and

$$\left.\frac{\partial n(\mathbf{r})}{\partial t}\right|_{\rm mb} = \sum_{\alpha_1\alpha_2} \phi_{\alpha_1}(\mathbf{r})\left.\frac{d\rho_{\alpha_1\alpha_2}}{dt}\right|_{\rm mb}\phi^*_{\alpha_2}(\mathbf{r}). \tag{8}$$

It is possible to show that, also for the simplest case of a semiconductor bulk system (whose single-particle states are momentum eigenstates: $\alpha = \mathbf{k}$), in the presence of a non-parabolic band, the single-particle evolution in Eq. (7) deviates from the classical diffusion term;[32–34] moreover, opposite to the Boltzmann theory, the scattering-induced variation in Eq. (8) is, in general, different from zero (see Figs. 1 and 2), i.e., the action of the proposed quantum-mechanical scattering superoperator (3) is spatially non-local, in clear contrast to the Boltzmann collision term.[35]

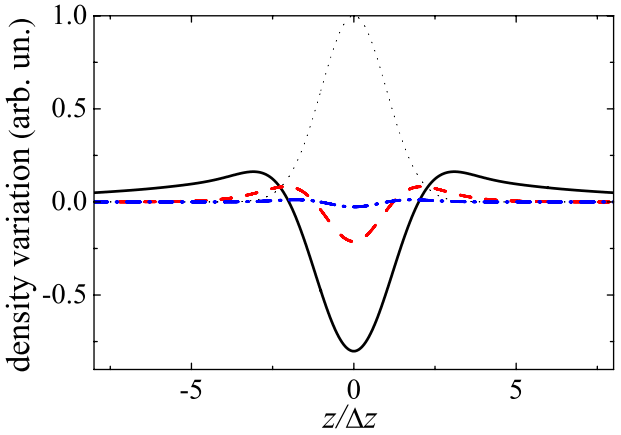

FIG. 1. Phonon-induced spatial non-locality in a GaAs bulk system: Initial time derivative of the spatial carrier density (see Eq. (8)) as a function of the relative coordinate z/Δ_z for three different values of the localization parameter: $\Delta_z = 5$ nm (solid curve), $\Delta_z = 50$ nm (dashed curve), and $\Delta_z = 200$ nm (dashed-dotted curve), together with the initial Gaussian density profile (dotted curve).

As stated in the fundamental solid-state text-book by Ashcroft and Mermin, a general and rigorous (i.e., quantum-mechanical) derivation of the standard semiclassical charge-transport theory constitutes a formidable task. The simplest approach to this tedious problem—usually referred to as the "diagonal limit"—is to neglect all non-diagonal density matrix elements, which implies to assume a single-particle density matrix of the form $\rho_{\alpha_1\alpha_2} = f_{\alpha_1}\delta_{\alpha_1\alpha_2}$.[36] By inserting such diagonal-limit prescription into Eqs. (1) and (3), it is easy to get the following equation of motion for the state population f_α:

$$\frac{df_\alpha}{dt} = \sum_s \sum_{\alpha'} [P^s_{\alpha\alpha'}f_{\alpha'} - P^s_{\alpha'\alpha}f_\alpha], \tag{9}$$

with $P^s_{\alpha\alpha'} = \mathcal{P}^s_{\alpha\alpha,\alpha'\alpha'}$. Equation (9) is Boltzmann-like, i.e., the time evolution of the carrier population f_α is dictated by a standard (in-minus-out) collision term involving scattering

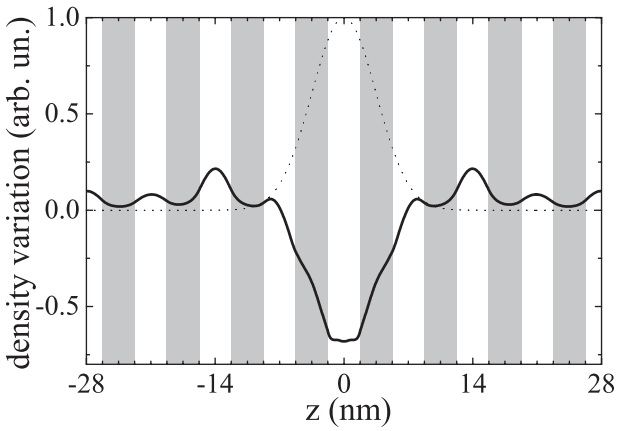

FIG. 2. Phonon-induced spatial non-locality in a GaAs/AlGaAs superlattice (band offset of 0.3 eV and well (GaAs) and barrier (AlGaAs) widths of 3.5 nm): Initial time derivative of the spatial carrier density (see Eq. (8)) as a function of the (absolute) coordinate z for an initial spatial localization of $\Delta_z = 3.5$ nm (solid curve) together with the initial Gaussian density profile (dotted curve).

rates $P^{s}_{\alpha\alpha'}$ given by the diagonal-approximation elements ($\alpha_1 = \alpha_2$ and $\alpha'_1 = \alpha'_2$) of the generalized scattering rates in Eq. (4). Indeed, Eq. (9) can be regarded as the formal justification and starting point of the wide variety of Monte Carlo simulations of semiconductor nanodevices previously recalled.[18–27] As anticipated, such diagonal-limit treatment is not able to properly describe the time-dependent evolution of the spatial carrier density; indeed, by inserting the diagonal prescription into Eq. (7), the single particle contribution to the spatial carrier density is always equal to zero, which implies that such a treatment does not allow one to account for the diffusion dynamics of the semiclassical theory. Moreover, within the diagonal approximation, the scattering-induced variation in Eq. (8) comes out to be totally non-local, in clear contrast to the Boltzmann collision term. Such highly unphysical behavior can be easily understood noticing that within the diagonal approximation the spatial carrier density in Eq. (5) reduces to

$$n(\mathbf{r}) = \sum_{\alpha} |\phi_{\alpha}(\mathbf{r})|^2 f_{\alpha}. \tag{10}$$

This tells us that for the particular case of a bulk system—the one considered in the derivation of the Boltzmann transport equation—the single-particle states are momentum eigenstates ($\alpha = \mathbf{k}$) whose probability densities $|\phi_{\alpha}(\mathbf{r})|^2$ are space-independent. It follows that in this case the diagonal-approximation carrier density in Eq. (10) is space-independent as well.

Opposite to the anomalous behavior just recalled, we shall show that the proposed density-matrix treatment (i) in the classical limit is able to well reproduce the local character of the scattering dynamics, and (ii) in the presence of a spatial carrier localization on the nanometric scale, it displays genuine non-locality effects. To this end, we have considered an effective one-dimensional ($\mathbf{r} = z$) GaAs-based nanostructure,[37] assuming for all the simulated experiments an initial density matrix corresponding to a spatial Gaussian carrier distribution

$$n(z) \propto e^{-\frac{z^2}{2\Delta_z^2}}, \tag{11}$$

as well as to a corresponding Gaussian distribution in the momentum space k, where Δ_z describes the degree of spatial localization of our initial state and $\Delta_k = \frac{\sqrt{m^* k_B T}}{\hbar}$ describes the thermal fluctuations of our carrier gas (m^* denoting the carrier effective mass).[38] As prototypical energy-dissipation/decoherence mechanism, we have considered carrier scattering due to acoustic phonons via deformation-potential coupling.[6]

Our first set of room-temperature simulated experiments corresponds to a GaAs bulk system (i.e., no confinement potential profile) and is displayed in Fig. 1. Here, we report the initial time derivative of the spatial carrier density (see Eq. (8)) as a function of the relative coordinate z/Δ_z for three different values of the localization parameter Δ_z. As we can see, in the presence of an initial nanometric confinement (solid curve), the phonon-induced time variation is significantly different from zero; the latter displays a negative peak corresponding to a replica of the initial distribution (so-called out-scattering contribution induced by the last term in Eq. (3)), and more importantly, a positive contribution extending over a much larger range (so-called in-scattering contribution induced by the first term in Eq. (3)). This is exactly the signature of scattering-induced spatial non-locality we were looking for. By increasing the value of Δ_z (dashed and dashed-dotted curves), the magnitude and relative spatial extension of such non-locality effects are significantly reduced, thus, confirming that in the classical limit $\Delta_z \to \infty$ the scattering-induced time variation tends to zero, as predicted by the conventional Boltzmann theory.

Our second set of room-temperature simulated experiments corresponds to a conventional GaAs/AlGaAs superlattice and is displayed in Fig. 2. Here, we report again the initial time derivative of the spatial carrier density (see Eq. (8)) as a function of the (absolute) coordinate z for an initial spatial localization of $\Delta_z = 3.5$ nm (solid curve) together with the initial Gaussian density profile (dotted curve). As we can see, also in the presence of the superlattice confinement potential, the phonon-induced time variation corresponding to an initial nanometric carrier localization is significantly different from zero, displaying again a negative peak corresponding to a replica of the initial distribution and a positive contribution extending over a much larger range. However, the presence of the semiconductor nanostructure gives rise to a non-trivial interplay between the spatial quantum confinement dictated by the nanostructure potential and the scattering-induced diffusion, resulting in a superlattice-induced modulation of the density variation (solid curve in Fig. 2). We stress once again that the investigation of such space dependent phenomena—not possible via Boltzmann-like Monte Carlo simulation schemes—constitutes a distinguished feature of the proposed quantum mechanical treatment.

To summarize, in this letter, we have proposed a conceptually simple and physically reliable quantum-mechanical generalization of the conventional Boltzmann theory able (i) to preserve the computational power and flexibility of the semiclassical picture in describing a large variety of interaction mechanisms, and (ii) to properly model space-dependent ultrafast phenomena, including non-locality effects leading to scattering-induced quantum diffusion. The proposed microscopic-modeling strategy bridges the gap between conventional (i.e., classical-like) Monte Carlo simulations and highly expensive quantum-kinetic approaches, and may play an important role in the investigation of ultrafast electro-optical processes in new-generation nanomaterials and nanodevices.

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[35]Indeed, by denoting with $\mathbf{r}, \mathbf{k}$ the semiclassical phase-space, the Boltzmann collision term[6] is local in space, since in any scattering process one deals with a momentum transfer without changing the carrier coordinate: $\mathbf{r}, \mathbf{k} \rightarrow \mathbf{r}, \mathbf{k}'$. It follows that, regardless of the specific interaction mechanism involved, the scattering-induced time variation of the spatial carrier density is always equal to zero: $\frac{dn(\mathbf{r})}{dt}\big|_{mb} = 0$.
[36]From a physical point of view, this amounts to assuming that the impact of various energy dissipation/decoherence phenomena (described via the scattering superoperator (3)) is so strong to suppress at any time all interstate ($\alpha_1 \neq \alpha_2$) quantum-mechanical phase coherence.
[37]More specifically, the single-particle states α of our semiconductor nanostructure are described via the standard envelope-function and effective-mass approximations[13] in terms of a plane-wave expansion.
[38]It is possible to show that at room temperature the uncertainty principle imposes the following restriction: $\Delta_z \geq \frac{1}{2\Delta_k} \simeq 3$ nm.