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Introduction

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The continuous downscaling of electronic devices has led to remarkable broadening of applications during the last twenty years, from nanoelectronics through the photovoltaics and more recently quantum computing.

Although these devices have reached nanodimensions, with carrier transport approaching the ballistic limit in the active region, it is widely recognized that inelastic scattering have still a significant influence. For instance, it has been shown theoretically that electron–phonon scattering drastically influences the current characteristics in ultimate nanowire transistors [1]. The miniaturization tends to enhance also the impact of thermal effects, and accurate description of phonon scattering at the nanoscale is becoming crucial to understand and manage thermal dissipation in devices and circuits [2]. In modern optoelectronic devices like new generation solar cells, it is also essential to consider appropriate models of light–matter interaction at the microscopic level [3,4]. Time-dependent quantum transport models are becoming more and more relevant to correctly assess and predict the properties of electronic quantum computing devices. In such devices, the energy of an electron can change during its travel across the active region and time-dependent modeling techniques are essential to predict their physical behavior [5].

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It then appears obvious that the development of emerging devices in nanoelectronics and optoelectronics requires sophisticated quantum transport simulations that can properly capture the properties of inelastic scattering.

Several theoretical approaches have been elaborated and improved during the last decade, and we aim at reviewing them within a dedicated issue of Journal of Computational Electronics.

The goal of this Special issue is thus to emphasize the recent developments in the area of quantum treatment of inelastic interactions in nanosystems including electron–phonon, electron–photon, electron–electron, phonon–phonon scatterings and time-dependent phenomena.

Among the recently developed quantum transport methods, the nonequilibrium Green's function (NEGF) formalism represents one of the most sophisticated and accomplished [6,7]. The great advantage of the approach is its capacity to model the inelastic interactions through the concept of self-energies [8–10]. The self-energies are added to the Hamiltonian of the active region and result from a subtle summation of Feynman diagrams of a given order in the considered interaction. They depend on the Green's functions which in turn are expressed as a function of the scattering self-energies [11]. Therefore, calculations of the scattering self-energies and the interacting Green's functions usually rely on a self-consistent scheme called the "self-consistent Born approximation" (SCBA). Alternative direct (i.e., not self-consistent) techniques [12–15] have been recently developed to calculate the scattering self-energies, but for the sake of clarity, they will not be addressed in this special issue.

Although formally implementable, the calculation of the scattering self-energies then induces a significant increase of the numerical burden due to the required self-consistency. The first set of papers propose NEGF code improvements for transistor modeling. The work of Mil'nikov and Mori shows

a novel equivalent transport model to realize NEGF atomistic simulations (i.e., using a tight-binding Hamiltonian for electrons and the valence force field scheme for phonons). The authors then calculate the electron–phonon scattering matrix elements in the spirit of random matrix theory. This technique allows them to implement an atomistic description of the device including phonon scattering with a moderate computational complexity. The approach is validated by calculating the phonon-limited mobility and current characteristics of Si nanowire metal-oxide-semiconductor field effect transistors (MOSFETs). Using a similar NEGF atomistic code (called "NEMO5"), the group of Klimeck at Purdue University investigates the transport in tunneling FETs. In particular, the co-workers assess the importance of the usually neglected real part of the electron–phonon self-energy. The authors also discuss the numerical optimization of such self-energy in the code. The next two papers are based on the NEGF approach in which the Hamiltonian is expressed either in the effective mass approximation or within the k.p method. In both works, bulk deformation potentials are used to describe the interactions between electrons and phonons. Martinez and co-workers first analyze the impact of phonon scattering in Si, GaAs, and InGaAs nanowire n-type MOSFETs. They investigate the influence of phonon scattering on the electron relaxation and show that a small amount of electronic power is dissipated into the active region of the device, which might lead to a strong self-heating. The authors also emphasize the importance of considering the real part of the phonon scattering self-energy to calculate the phonon-limited mobility in the on- and the off-regimes. The second paper is from Pala et al., which studies the impact of phonon scattering in tunnel FETs. Since tunnel FETs work at low supply voltage, the impact of phonon scattering is negligible in the on-regime. The authors then focus on the off-regime of InAs nanowire tunnel FETs and 2-D vertical tunnel FETs based on metal dichalcogenide heterojunctions, which are very promising candidates. In particular, the authors investigate the processes of phonon-assisted transport phenomena through the presence of traps in the band-gap.

The modeling of nanoscale photovoltaic devices adds another difficulty to the problem since electron–photon interactions must also be incorporated. Electron–photon interactions can be implemented through the "standard" self-consistent Born approximation but this time by considering two self-energies, since phonon scattering is still to be included. Aeberhard first focuses on the capacities of the NEGF formalism to describe the main physical processes occurring in nanostructured solar cells. In particular, he investigates the numerical properties of the NEGF code convergence when including simultaneously electron–photon and electron–phonon interactions. He tested the SCBA scheme to study several phenomena like optical transitions, intraband transitions, phonon-assisted absorption, carrier escape etc. The conclusions show that the convergence speed of the SCBA current depends principally on the carrier localization more than the interaction strength. Still in the context of NEGF photovoltaic simulations, Cavassilas and co-workers analyze the impact of the usually assumed local approximation to calculate the electron–photon self-energy. Indeed the locality of the self-energy is required to use the efficient recursive algorithm to calculate the Green's functions. The authors then analyze the impact of nonlocality of the electron–photon self-energy in three different configurations: considering either a bulk flat band, a double dot solar cell with a monochromatic illumination, and a more realistic system in which the black body spectrum or a non-zero electric field are considered. The results tend to demonstrate that the importance of nonlocality in the electron–photon self-energy is reduced in such realistic situation.

Finally, time-dependent simulations become fundamental for the study of disruptive electronic quantum devices for quantum computing applications. Weston and Waintal then showed that time-resolved simulations of quantum devices can be performed using elementary bricks of Green's functions. In the present paper, they propose a numerically efficient method called the "source–sink algorithm" and apply it to the study of a charge pulse injected into an interferometer to obtain a flying qubit.

Another formalism of quantum transport is based on the Wigner function which is defined in the phase space as a Fourier transform of the density matrix [16]. This function is thus the quantum counterpart of the semiclassical Boltzmann distribution function. The resulting Wigner transport equation (WTE) shares many similarities with the Boltzmann transport equation (BTE) to such a point that the semi-classical limit of the WTE is nothing but the BTE [17]. Different methods have been developed to solve the WTE, including direct solutions [18,19] and particle Monte Carlo algorithms [20–22], in strong analogy with what has been developed in the past for solving the BTE. It has been recently extended to treat time-dependent ab initio simulations as well as many-body quantum problems and entangled systems [23,24]. The analogy between Boltzmann and Wigner formalisms is so strong that to consider the scattering effects in the Wigner approach of quantum transport it has been shown that the Boltzmann collision operator, based on the Fermi golden rule to treat instantaneous scattering events, is usually a very good approximation [25,26]. This approximation leads to the so-called Wigner–Boltzmann transport equation, which has been successfully used to solve many problems. In particular, it is an ideal tool to bridge the gap between diffusive semi-classical transport and fully coherent quantum transport [27].

However, in a paper of this issue, Zhan and co-workers point out that the use of the Boltzmann collision operator in quantum simulation may produce unphysical results when

the initial states before the collision are different from the additional states generated by the collision operator. This inconsistency may lead to negative values of the charge density, which disappears when the collision operator generates states that were present in the density matrix of the system before the collision. The authors propose an algorithm able to fix this issue and to model properly the electron–phonon interaction, without leading to negative values of the charge density.

Wigger and co-workers make use of the Wigner transport formalism to study the quantum dynamics of optical phonons generated by optical excitation in a quantum dot. In particular, they discuss the effect of a finite duration of the excitation pulse. By calculating the fluctuation properties of the phonons, they show that phonon squeezing can be achieved by optical manipulation of the quantum dot exciton. The pulse duration appears to be a crucial parameter for this intriguing physical effect.

As an alternative to the Wigner formalism, it is possible to work with the density matrix itself to solve some quantum transport problems. Within the density matrix theory, the derivation of effective kinetic equations for the electronic gas in a quantum device may involve one of the following approximation or both: (i) the mean-field approximation and (ii) the adiabatic or Markov limit within which the memory effects are neglected [28]. The combination of these two approximations may lead to unphysical results, as negative distribution functions and nondissipative carrier–phonon coupling [29,30]. A proper combination of adiabatic limit and mean-field approximation is required to guarantee a physically acceptable solution [31]. However, when the system–environment coupling becomes strong and/or the excitation timescale is extremely short, Markovian approaches are known to be unreliable, and memory effects have to be taken into account via so-called quantum-kinetic schemes [7,32,33]. Hence, the derivation of non-Markovian treatments able to ensure the positive-definite character of the single-particle density matrix would be of high importance, but is still missing.

In their paper, Iotti and co-workers discuss the advantages and limitations of such non-Markovian density matrix approaches. By means of a two-level model, they show that severe limitations may arise in zero-dimensional electronic systems—like GaAs or GaN quantum dots, the potential constituents of quantum-computation devices—strongly coupled to dispersionless phonon modes. Jonasson and co-workers propose a computationally efficient density-matrix model based on a rigorously derived Markovian master equation. This approach conserves the positivity of the density matrix, includes off-diagonal matrix elements as well as full in-plane dynamics and time dependence, and accounts for the relevant scattering mechanisms with phonons and impurities. They apply this model to a quantum cascade laser (QCL) operating in the THz range. It is shown in particular that the magnitude of the off-diagonal elements of the density matrix can be a significant fraction of the diagonal values, demonstrating the importance of including coherences in describing QCLs. In addition, the analysis of time-resolved results gives insight into the response of the device to a suddenly applied bias, thus revealing the different time scales involved.

For further details on some aspects and methods of quantum transport simulation, the reader may refer to two recent Special Issues of J. Comput. Electron., i.e., the Special Issue on Quantum Transport Beyond DC (J. Comput. Electron., vol. 12 (3) 2013) and the Special Issue on Wigner Functions (J. Comput. Electron., vol. 14 (4) 2015).

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