Dissipative quantum transport using one-particle time-dependent (conditional) wave functions

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INTRODUCTION

A quantum device is a many-body open system driven far from (thermodynamic) equilibrium. For ballistic systems, these difficult proble is traditionally solved from the one-particle Schrödinger equation which only captures non-dissipative (elastic) scattering of electrons with external potentials. In principle, one would like to include dissipation into the previous one-particle wave functions of the electron. However, strictly speaking, such one-particle wave functions (for a quantum subsystem) do not exist in the Copenhagen formulation of quantum phenomena [1]. Thus, much less intuitive mathematical entities are required: the density matrix [2], its Wigner-Weyl transformation named Wigner distribution function [3] or the so-called non-equilibrium Greens function (NEGF) formalism [4]. Fortunately, the concept of one-particle wave function (of a quantum subsystem) including dissipation can be rigorously formulated within the Bohmian explanation of quantum phenomena [5].

ONE-PARTICLE CONDITIONAL WAVE FUNCTIONS

In this conference, we show how dissipation in quantum transport can be rigorously tackled from the (conditional) wave function, with the computational burden limited to solving one-particle wave functions with time-dependent potentials. Let us consider a many-particle wave function $\Phi(\vec{r},t)$ solution of the unitary Schrödinger equation where $\vec{r}=\{\vec{r}_a,\vec{r}_b\}$ with $\vec{r}_a$ the position of the $a-$electron and $\vec{r}_b=\{\vec{r}_1,....,\vec{r}_{a-1},\vec{r}_{a+1},....,\vec{r}_N\}$ the positions of the rest. Bohmian mechanics defines the so-called *conditional wave function* [1], [6] as:

$$\Psi_a(\vec{r}_a,t)=\Phi(\vec{r}_a,\vec{R}_b^{\alpha}(t),t), \qquad (1)$$

which constitutes a slice of the whole multi-dimensional wave function $\Phi(\vec{r},t)$. All degrees of freedom are substituted by Bohmian trajectories except $\vec{r}_a$. It has been demonstrated [6] that $\Psi_a(\vec{r}_a,t)$ obeys the following wave equation:

$$i\hbar\frac{\partial\Psi_a(\vec{r}_a,t)}{\partial t}=\Big\{-\frac{\hbar^2}{2m}\nabla_a^2+U_a(\vec{r}_a,\vec{R}_b^{\alpha}(t),t) +G_a(\vec{r}_a,\vec{R}_b^{\alpha}(t),t)+iJ_a(\vec{r}_a,\vec{R}_b^{\alpha}(t),t)\Big\}\Psi_a(\vec{r}_a,t). \qquad (2)$$

where the Bohmian trajectories are denoted by $\vec{R}(t)=\{\vec{R}_a^{\alpha}(t),\vec{R}_b^{\alpha}(t)\}$ with α an index for the possible initial positions [1]. The term $U_a(\vec{r}_a,\vec{r}_b^{\alpha}(t),t)$ can be any type of many-particle potential defined in the position-representation. The explicit expression of the potentials $G_a(\vec{r}_a,\vec{r}_b^{\alpha}(t),t)$ and $J_a(\vec{r}_a,\vec{r}_b^{\alpha}(t),t)$ can be found in reference [6]. It is important to specify that (2), contrarily to the orthodox Schrödinger equation, provides a non-linear and non-unitary evolution of the one-particle wave function $\Psi_a(\vec{r}_a,t)$ that allows the modeling of dissipation, decoherence and (collapse) measurement with minimum computational difficulties [7].

ELECTRON-PHONON INTERACTION

As an example, we consider the electron-phonon interaction in a typical AlGaAs resonant tunneling structure. In particular we consider emission and absorption of optical phonons with energy $\hbar\omega_{op}=0.03613\ eV$. The scattering rates are directly obtained from the Fermi Golden Rule. Under the assumption that the spatial dependence of the perturbing potential is smaller than its temporal dependence, it can be demonstrated that $J_a(\vec{r}_a,\vec{r}_b^{\alpha}(t),t)$ in (2) is negligible and $G_a(\vec{r}_a,\vec{r}_b^{\alpha}(t),t)$ can be easily approximated to satisfy the electron-phonon energy conservation. The initial (quantum ensemble) energy $\langle E\rangle$ of $\Psi_a(\vec{r}_a,t)$ is modified by $G_a(\vec{r}_a,\vec{r}_b^{\alpha}(t),t)$ until its final value $\langle E\rangle\pm\hbar\omega_{op}$. See figures 1 and 2 and the explanation therein.

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CONCLUSIONS

In this conference, we present a new formalism to study dissipative transport with one-particle (conditional) wave functions. This new feature has been included, as the last step, into the general, versatile time-dependent BITLLES simulator [8]. Previous features included into the BITLLES are electron-electron interaction beyond mean field [9], open system boundaries [10], exchange (fermion) interactions [11], [12], noise computation [7], [13] and high-frequency displacement currents [14]. This last ingredient, the quantum dissipation, clearly justifies why the BITLLES simulator is the natural (full) quantum extension of the Monte Carlo algorithm for the semi-classical Boltzmann equation, where the dynamics of the electron trajectories are guided by the one-particle (conditional) wave function discussed in (2) rather than by the electric field.

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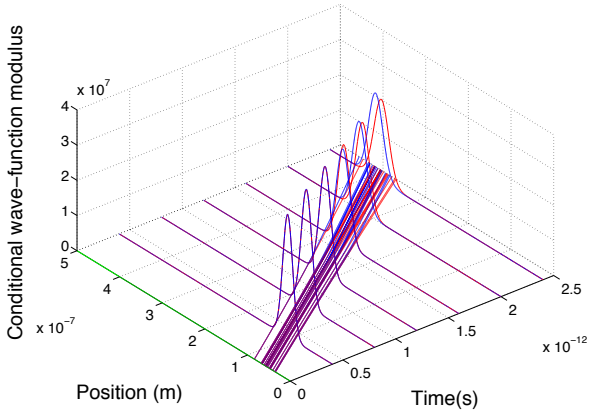

Fig. 1. (Red) Time-evolution of a wave function and associated trajectories solution of the one-particle Schrödinger equation and (Blue) Time-evolution of a (conditional) wave function and associated trajectories solution of the one-particle wave in (2) where the absorption of a phonon is considered. (Green) the free space potential. Initial wave packet energy $\langle E \rangle = 0.05eV$. The (blue) conditional wave function and its trajectories have a larger velocity (kinetic energy) than the (red) Schrödinger wave function after the interaction with the phonon. From a computational point of view, only a proper shape of the term $J_a(\vec{r}_a, \vec{r}_b^{\alpha}(t), t)$ in the time-dependent wave equation (2) is required to discuss dissipation.

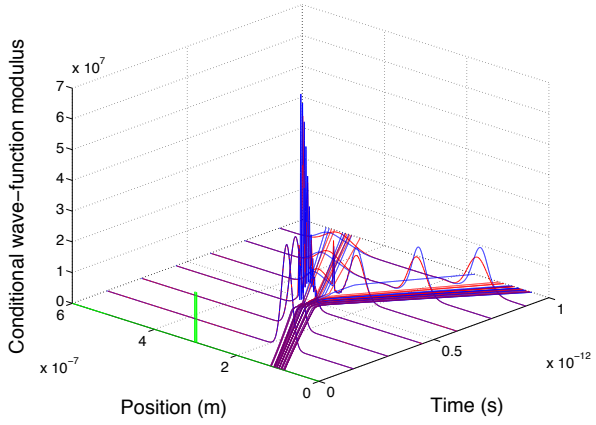

Fig. 2. The same data as in Fig. 1 for a double barrier 1nm/4nm/1nm structure plotted in green. Barrier height 0.3 eV. Initial wave packet energy $\langle E \rangle = 0.1eV$. The (blue) conditional wave function and its trajectories have a larger velocity (kinetic energy) than the (red) Schrödinger wave function after the interaction with the phonon. In addition, the interaction with the phonon slightly increases the number of reflected trajectories. This is due to the fact that the energy of the electron after interacting with the phonon deviates from the resonant energy.