Scattering implementation in the quantum transport BITLLES simulator

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Among the different implementations of scattering in the literature that allow to effectively account for the perturbation induced by the non-simulated degrees of freedom on the simulated ones, the direct implementation of the Fermi golden rule, developed to study transitions between an initially-prepared and a finally-measured pure state (see Fig. 1(a)), is the most simple and intuitive. However, describing pure state transitions inside the active region of a nanoelectronic device bears two important difficulties. First, open quantum systems cannot be represented in terms of pure states, except for Markovian processes. Second, in the transition from one pure state to another, some type of decoherent phenomena have to be added to break the unitary evolution of the system (See Fig 1(b)).

In this conference, we show that Bohmian conditional wave functions (CWFs) [1] allow a simple and rigorous way of implementing the Fermi golden rule transitions between pre- and post-selected pure states in open quantum systems both under Markovian or non-Markovian conditions [3] solving the two mentioned problems, as indicated in Fig.1(d). We discuss the practical application of the method for light-matter interaction, with emission/absorption of photons in double barrier structure of a Resonant Tunneling Device (RTD). As a practical discussion, we study Model A where the final CWF is post-selected by increasing/decreasing the initial energy of the pre-selected CWF (satisfying overall energy conservation), and Model B where such transition is done with the mean momentum increased/decreased. Such Model B is only valid for flat potential conditions where energy and momentum operators commute. For arbitrary potentials, as the double barrier considered here where energy and momentum do not commute, Model B leads to unphysical scattering processes without energy conservation (see fig. 2(b)). These unphysical features are clearly seen in the oscillatory behavior of the CWF in Fig. 3(c) when photon absorption is considered. On the contrary, Model A perfectly captures the physics of the absorption (and spontaneous emission not plotted) as seen in Fig. 3(b), which becomes relevant phenomena for high frequency (THz) quantum transport [5].

This scattering process between pre- and post-selected CWF, within Model A, provides the last ingredient for the BITLLES simulator [4] to become a general purpose, versatile and intuitive quantum transport simulator ready for the electronic industry.

[1] X. Oriols and J. Mompart, Jenny Stanford Publishing: Singapore, (2019)

[2] D. Pandey et al., Entropy, **21,** 12, 1148 (2019)

[3] M. Villani et al., IEEE EDL, **42**, 2, 224-227, (2021)

[4] The BITTLES simulator. Available online: http://europe.uab.es/bitlles.

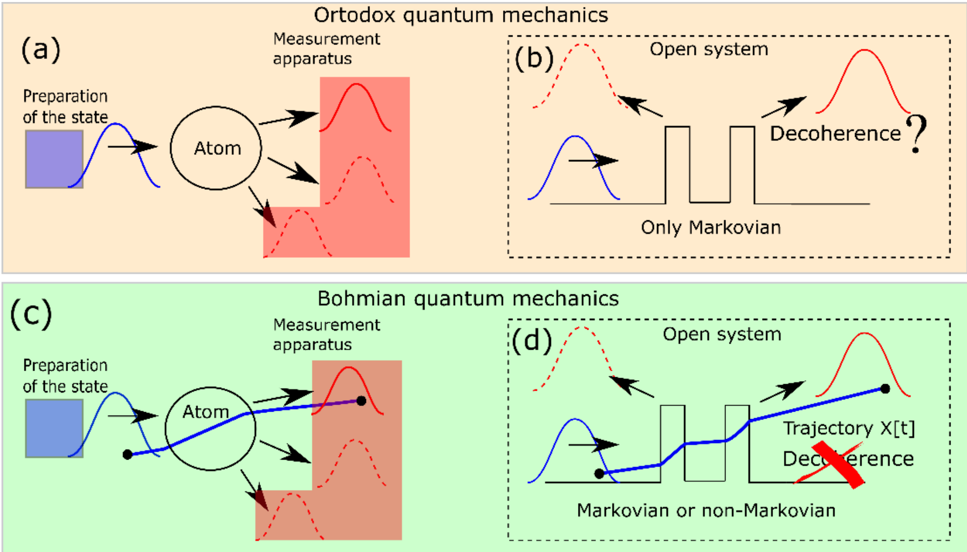

Figure 1: Schematic representation of the Fermi Golden rule from orthodox quantum mechanics in (a) and (b), and from Bohmian quantum theory in (c) and (d). The preparation and measurements of pure states in closed system, (a) and (c), is unproblematic, while in open system is problematic in (b) with pure states, but not in (d) with conditional wave functions.

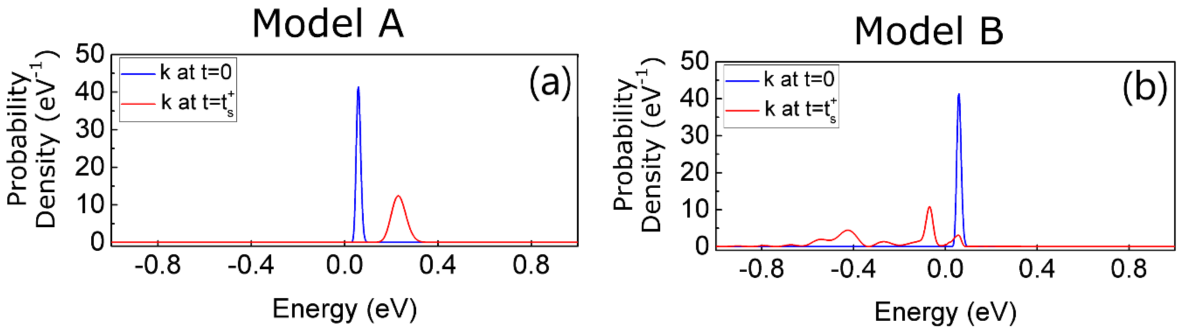

Figure 2: Evolution of the probability density of the CWF components due to photon absorption with Model A in (a) and Model B in (b). Blue lines denote the probability distribution before the scattering, while red lines after it.

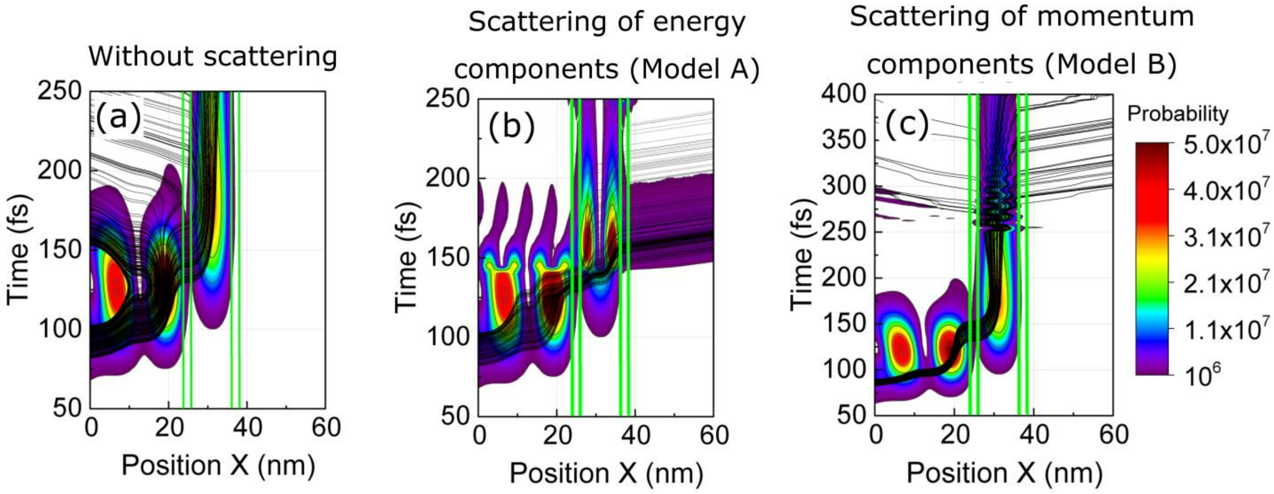

Figure 3: Evolution of the CWF and the Bohmian trajectories X[t] in space and time. (a) without photon absorption, (b) with photon absorption using model A, (c) with photon absorption using model B. In (b) the CWF transition from the first to the second resonant level of the quantum well is clearly seen (Model A), while in (c), unphysical oscillations appear (Model B).