Quantum simulation of 2D materials with dissipation

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Dissipation is always present in electron devices. It is a direct consequence of time-irreversible processes whose proper simulation, in quantum systems in general and in 2D materials in particular, has always been a challenging task. In this work, we present a new formalism that accounts for the interaction of electrons with other degrees of freedom in 2D materials (e.g. phonons or photons) by just including a new *potential* term into the Dirac Hamiltonian.

Electron devices are *naturally* defined in the physical space. Therefore, the great advantage of our approach, based on the use of the conditional wave function [1, 2], is that it introduces dissipation and many-body physics [1] in a rigorous and transparent way, directly into the physical space, rather than in more abstract mathematical spaces (like Fock space, phase-space, etc). In Fig. 1 and 2, we plot an electron travelling in a graphene sheet, while interacting with a phonon. The presence probability (color map) and its ray interpretation associated to Bohmian trajectories (black lines) [1,3] are depicted.

We emphasize that this new powerful approach is suitable for any system which exchanges energy or momentum with a subsystem, thereby making it an excellent and ideal simulation tool [3] for dealing with dissipation and time-irreversible dynamics in any other quantum research field.

References
[1] X. Oriols, PRL, 98 (2007) 066803
[2] D. Marian, N. Zanghì, and X. Oriols, PRL, 116 (2016) 110404
[3] http://europe.uab.es/bitlles

Figures:

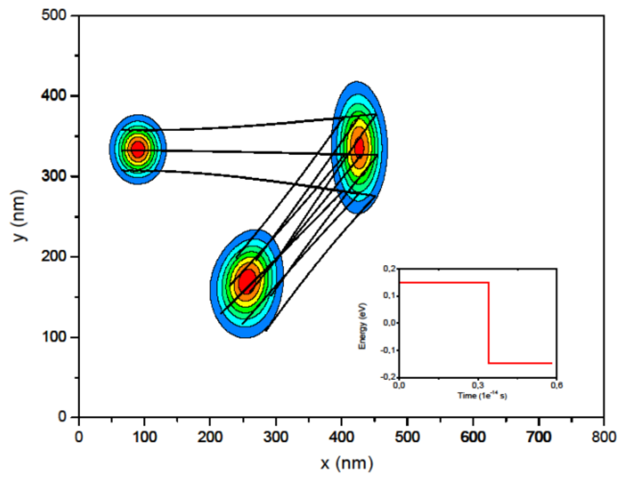

Figure 1: An electron, due to the interaction with a phonon, makes a transition from the conduction band to the valence band changing its momentum and energy. Inset: time-evolution of the total electron energy.

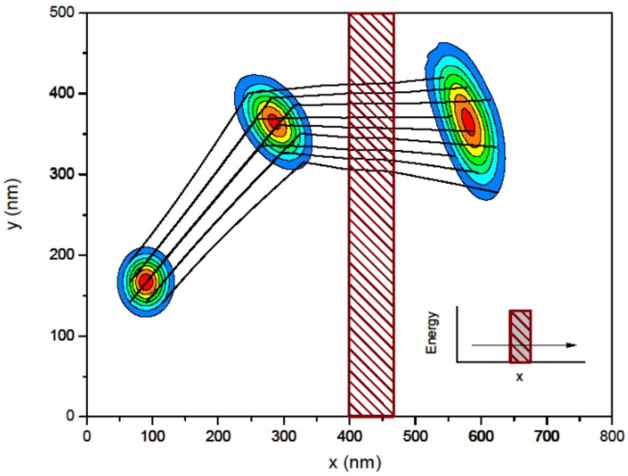

Figure 2: An electron is kicked by a phonon, changing its momentum, and then impinging perpendicularly to the barrier (oblique lines). Thus, Klein tunnelling occurs and the electron transmission is maximized. Inset: electron (arrow) and barrier energy (oblique lines) profile.