Weak values: a new paradigm to characterize nanoscale systems

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INTRODUCTION

Since their introduction more than 30 years ago, weak values are gradually transitioning from a theoretical curiosity to a practical tool in both, physical and computational experiments, allowing an unprecedented characterization of quantum systems. Weak values can provide information of quantum systems beyond those provided by the traditional expectation or correlation values of Hermitian operators. As such, they open an unexplored paradigm to give experimentally meaningful microscopic properties to nanoscale systems in computational simulations. Several examples will be presented in this workshop [1-5].

EXPERIMENTAL AND THEORETICAL WEAK VALUES

From the experimental point of view, the weak value is a complex number that can be obtained in the laboratory through a well-defined operational protocol, consisting in a weak measurement of a property plus a subsequent strong measurement of another property, for an ensemble of identically prepared quantum systems $|\Psi\rangle$. The novelty of the weak values appears when such measured properties belong to non-commuting operators [3]. From a theoretical point of view, when for example, the first (weak) measurement is of the momentum linked to the operator $\hat{p}$, and the second (strong) measurement is of the position x, the weak value is defined as

$$p(x) = \langle \mathrm{x}|\hat{p}|\Psi\rangle/\langle x|\Psi\rangle \ ,$$

which can be interpreted as a distribution of momenta along the position x. This weak value turns out to coincide with the (Bohmian) velocity in Bohmian theory [3]. In fact, the computation of momentum weak values (post selected in position) appears quite naturally in different formulations of quantum hydrodynamics.

NOVEL CHARACTERIZATION OF NANOSCALE SYSTEMS

In this workshop, we will present several examples where these weak values allow the computational simulation (and thus prediction) of empirical properties of nanoscale systems, that were seemingly inaccessible from standard expectation or correlations values. Among others, they allow:

(i) A natural extension of the classical Monte Carlo technique for electron transport to quantum systems through well-defined trajectories [1]. See Fig. 1.

(ii) Pure-state "unravellings" in non-Markovian open quantum systems, using conditional states [4].

(iii) A non-contextual definition of the quantum work operator for quantum thermodynamics [3], and of two-time correlations for non-commuting observables [3].

(iv) The computation of the dwell-time in the active region of nanoscale devices [2] (see an example for graphene in Fig 2).

(v) The understanding of quantum thermalization of many-body systems, by distinguishing two components of the kinetic energy [5]. See Fig. 3.

CONCLUSION

Weak values allow us to simulate new practical properties that can be later tested in the laboratory. As such, we argue that they will become essential tools for computational nanotechnology in the forthcoming years.

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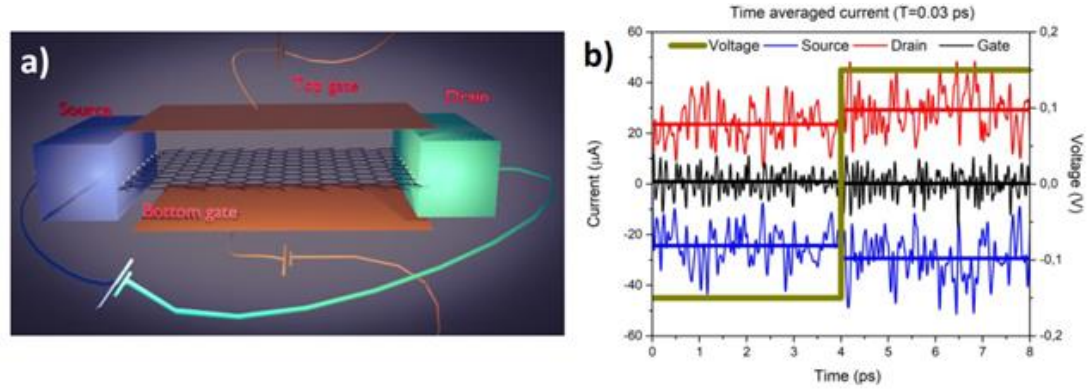

Fig. 1: (a) Schematic representation of the graphene-based FET, with a channel composed of a single-crystal monolayer graphene. (b) The high frequency lines are the instantaneous currents (time-averaged at a window of 0.03 ps) as a function of time, computed from the dynamics of Bohmian trajectories. The straight lines are due to a wider averaging window of 4 ps, where we can clearly assert the binary response. We can conclude that 4 ps is a reasonable operating time for the transistor.

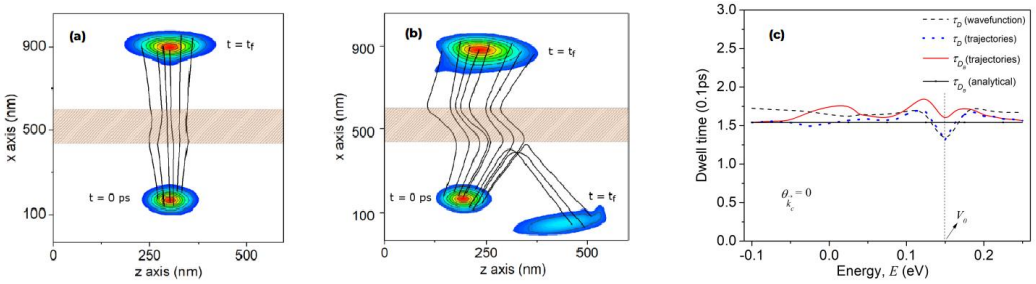

Fig. 2: A conditional wave packet in graphene impinges upon a barrier (shaded orange region) suffering Klein tunneling with an incident angle of zero degrees (a) and 15 degrees (b). The ability to use trajectories allows us the unambiguous definition of the dwell time of electrons in graphene, as seen in (c) for the incident angle of (a) as a function of the central energy of the wave packet. Such a time, unambiguously computed from measurable weak values, directly determines the high frequency behavior of nanoscale devices.

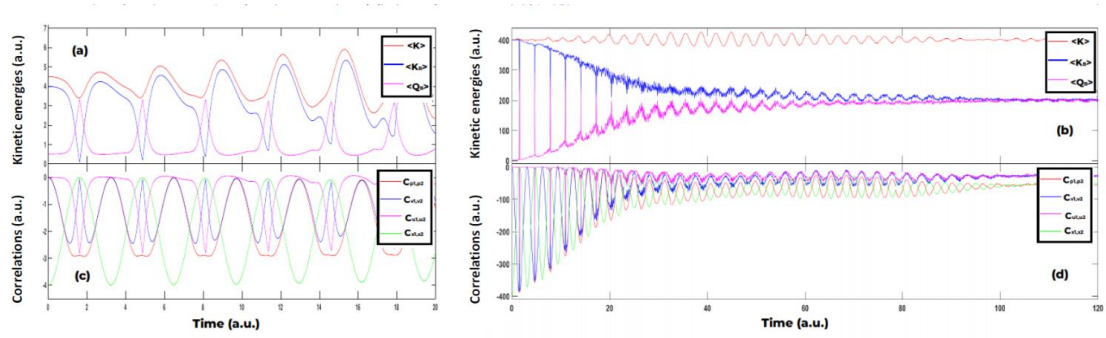

Fig. 3: (a) Expectation and correlation values of the dynamics of two particles in an harmonic trap. Left panels: a few initial cycles under no disorder showing a periodic behavior; Right panels: whole dynamics under disorder showing thermalization. Panels (a), (b) for kinetic energies comparison: Orthodox ⟨K⟩, Bohmian ⟨KB⟩, quantum potential ⟨QB⟩ energies. Panels (c), (d) for correlations: momentum Cp1,p2, Bohmian velocity Cv1,v2, osmotic velocity Cu1,u2, position Cx1,x2 correlations. The result ⟨K⟩/2= ⟨KB⟩=⟨QB⟩ is a signature of thermalization, even when ⟨K⟩ is constant, that can only be accessed through weak values.