Quantum many-particle computations with Bohmian trajectories:
Application to electron transport in nanoelectronic devices

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From a computational point of view, the solution of a system of N interacting particles is inaccessible because it requires solving the many-particle Schrödinger equation in the huge configuration space associated to the N particles. It has been demonstrated [1] that a system of N interacting particles can be decomposed into N single-particle (pseudo) Schrödinger equations coupled by Bohmian trajectories. The proposal has similarities with the original work of Kohn and Sham [2] on the Density Functional Theory (DFT). The formidable simplification on the many-particle computations comes at the price that some terms of the potential energy of the corresponding single-particle Schrödinger equations are unknown (the exchange correlation functional in the DFT and a complex potential energy in [1]).

In particular, the previous algorithm [1] has been used to develop a powerful quantum (Monte Carlo) simulator of electron transport for nanoelectronic devices (in time-dependent, open systems and far from equilibrium scenarios). Within standard computing facilities, the present proposal is able to deal with N<100 electrons with Coulomb and exchange interactions. Numerical computations of the electron-electron correlation effects on the DC, AC and current noise in resonant tunneling devices are presented [3,4].

References:
[1] X.Oriols, Phys. Rev. Lett. 98, 066803 (2007).
[2] W.Kohn and L.Sham, Phys. Rev. 140, A1133 (1965).
[3] A.Alarcon and X.Oriols, J. Stat. Mech. P01051 (2009).
[4] G.Albareda, J. Suñé and X. Oriols, Phys. Rev. B 79, 075315 (2009).