Exploring Neural Networks for Predicting Bohmian Trajectories in Many-Body Scenarios

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The conventional approach to solving the many-body problem in quantum mechanics, which involves predicting the behavior of a system comprising N interacting particles, typically entails substituting the many-body wave function in configuration space with a coupled system of N single-particle wave functions, each defined in physical space. Density Functional Theory (DFT) stands out as the most prominent and successful example of this strategy. Similarly, within the framework of Bohmian mechanics, a natural path to define a wave function of a quantum subsystem is offered through the use of conditional wave functions [1]. However, in both approaches, a major challenge lies in precisely defining the equation of motion for such single-particle wave functions, particularly in determining the exact single-particle potentials required to obtain exact solutions.

Recently, within the realm of DFT, artificial intelligence algorithms have gained widespread adoption within the scientific community to train computers to discern the appropriate single-particle potentials in well-known scenarios, enabling the computer to autonomously predict potentials in unknown scenarios.

In this conference, we delve into a similar strategy for Bohmian conditional wave functions. Our aim is to investigate the feasibility and implications of utilizing neural networks to model and predict Bohmian trajectories in many-body scenarios. Specifically, in this preliminary study, we solve in an exact way a light-matter system consisting of one electron and one mode of the electromagnetic field in the strongly interacting regime [2], resulting in Rabi oscillations as depicted in Figure 1. Various trajectories, conditional wave functions, and profiles of single-particle potentials are then utilized to train a computer to be able to anticipate the potential profile required for a new trajectory that has not been computed before. Figure 2 illustrates the comparison between the exact Bohmian trajectory, and the one obtained from extrapolating known potentials from other trajectories. Despite much more work is needed to get definitive conclusions about the computational adavatnages, this preliminary work indicates the feasibility of using artificial intelligence algorithms to the resolution of the many-body problem within the framework of Bohmian mechanics [3].

References

[1] X. Oriols, "Quantum-trajectory approach to time-dependent transport in mesoscopic systems with electron-electron interactions" Phys. Rev. Lett. 98, 066803 (2007).

[2] Carlos F. Destefani, Matteo Villani, Xavier Cartoixa, Michael Feiginov, Xavier Oriols "Resonant tunneling diodes in semiconductor microcavities: modeling polaritonic features in the THz displacement current" Phys. Rev. B 106, 205306 (2022).

[3] C. F. Destefani and X. Oriols "Kinetic energy equipartition: a tool to characterize quantum thermalization" Phys. Rev. Research, 5, 033168 (2023).

Figures

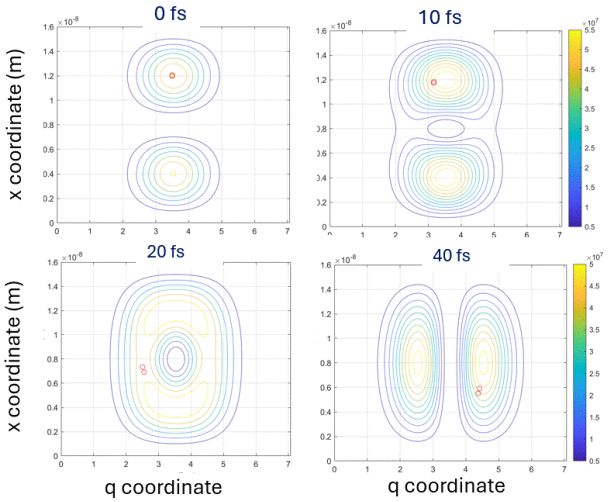

Figure 1. Time evolution of the 2D wave function (contour) and Bohmian trajectories (red circle) for an electron (x) and electromagnetic mode (q) in the strong light-matter regime, showing Rabi oscillations.

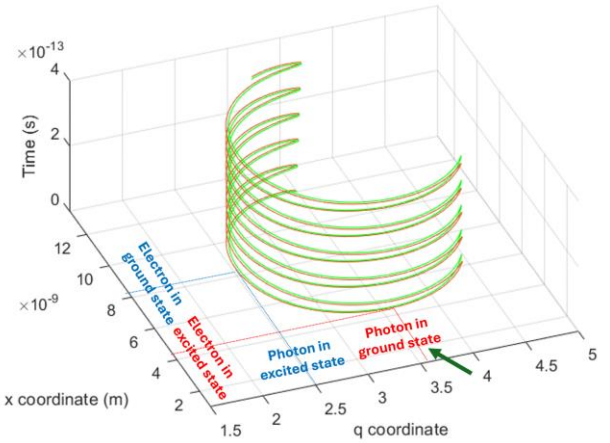

Figure 2. Time evolution of the (green) exact Bohmian trajectories from a 2D wave function of figure 1 and (orange) approximate Bohmian trajectory from a 1D conditional wave function with a 1D potential interpolated from the knowledge of other exact trajectories.