Fast Non-Adiabatic Warm Dense Matter Simulation

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When constructing modern simulations of Warm Dense plasma, one must make compromises in accuracy so that the calculations are computationally accessible. One of the many difficulties inherent in these simulations is the vast difference in the time scales of electron and ion motion. To access long-time ion correlations, then, the Born-Oppenheimer approximation is usually relied upon so that simulations can be performed at the time scale of the ions[1,2].

However, the neglect of electron dynamics associated with the Born-Oppenheimer approximation has been shown to produce systematic errors in the ion dynamics, and hence the ion-ion dynamic structure factor, that are difficult to quantify and correct[3]. Further, existing non-adiabatic/non-Born-Oppenheimer approaches require significant computational expense, to the point that they can become impractical for calculating long-term ion correlations[4].

Here, we present a new simulation method for modelling the dynamics of quantum plasmas that goes beyond the Born-Oppenheimer approximation, by treating electrons and ions as thermally-averaged Bohmian trajectories. Beginning with the standard description of Bohm's theory of quantum mechanics[5], we systematically construct a set of classical trajectories capable of accurately reproducing static and dynamic properties of Warm Dense Matter.

Our method complements existing state of the art Density Functional Theory methods. Due to a greatly reduced computational expense, we are able to treat long-time ion dynamics of large systems while also treating electrons fully dynamically. We thereby fill a void where current methods require a prohibitive computational cost.

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