Interacting trajectory representation of ultrafast quantum dynamics

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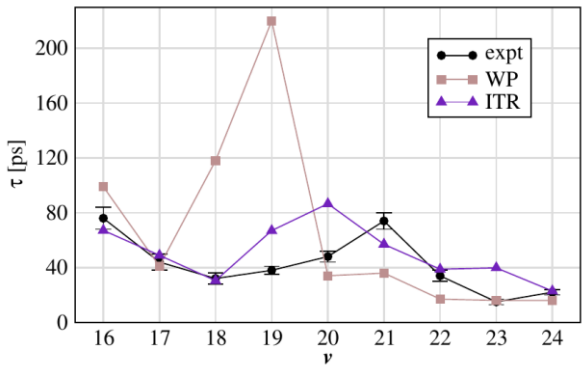
ABSTRACT

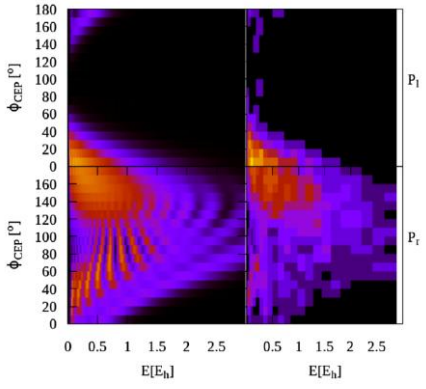
We present a general methodology to perform quantum dynamical simulations based on interacting trajectories without reference to any wave function, where the effect of the quantum potential is mimicked by effective pseudo-particle interactions. The method is applied first to several model quantum systems, both for bound and scattering problems. For the bound systems, the quantum ground state density and zero point energy are shown to be accurately computed within the interacting trajectory representation (ITR). In the case of time-dependent quantum scattering, the transmission coefficients are found to be in very good agreement with standard quantum calculations. Finally, we show that via wave function synthesis along the trajectories, correlation functions and energy spectra can be obtained based on the dynamics of interacting trajectories [1].

The method is applied subsequently to different test cases, namely the ultrashort laser ionization of a model hydrogen atom [2], the vibrational predissociation of a triatomic van der Waals complex [3],and the photoexcitation of alkali metal atoms embedded in rare gas matrices. We show that the trajectory-only approach is capable of correctly describing the large amplitude motion and energetics of the laser driven electron and of reproducing carrier-envelope phase (CEP) effects onto the photoelectron spectra. In addition, the predictions of the present methodology are in very good agreement with the available experimental data for the vibrational predissociation rates and the absorption spectra of the target systems. It also provides an intuitive picture of the dynamical quantum processes involved.

Lifetimes of the predissociating $ArBr_2(B,v)$ vdW complexes



Effect of the CEP on the photoelectron spectra



References

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