

Semiclassical initial value representation with complex trajectories

Adriano Grigolo
Universidade Estadual de Campinas

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Resumo

Semiclassical time-dependent solutions to the Schroedinger equation can be obtained by use of integral formulas known as initial value representations (IVRs). Over the last few decades IVR formulas have established a sucessful reputation, most notably in the field of physical chemistry, for it is often found that the quantum behavior of molecular systems is very well approximated by semiclassical wavefunctions. The IVR input consists in a swarm of independent classical trajectories, each of which obeys the dynamics dictated by the system's unquantized Hamiltonian. In a recent work [Aguiar et al, Chem. Phys. 370 (2010)] an IVR expression based on complex classical trajectories was formulated. The complex nature of the classical trajectories in this particular formula is a consequence of employing minimum uncertainty wavepackets (coherent states) to represent the time evolution operator upon which the formula is constructed. Here, an improved and simpler version of this complex IVR formula is presented. In order to test its accuracy, we apply it to a simple model system.