Semi-classical Nuclear-Phase Approach to Calculating Reaction
Cross-Sections

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Abstract

I propose a new *ab initio* method of calculating scattering cross-sections for use with Electron-Nuclear Dynamics (END) trajectories to replace the Schiff formulation[1]. After a bundle of trajectories is obtained from the dynamics, the nuclear phase of each trajectory is followed out to a common distance from the scattering center according to $\Phi = \int_{\vec{r}(t)} \vec{k} \cdot d\vec{x}$ where $\vec{r}(t)$ is the current trajectory. The value of the phase on the defined (asymptotic) spherical surface is then used to solve the asymptotic Schrödinger equation on that sphere. The resulting semiclassical wavefunction forms a direct approximation to the scattering amplitude, from which the cross-section can be derived in the usual fashion.

Much work remains to be done before this method is usable; remaining challenges include how to deal with rainbow and glory angles in a systematic fashion. I am currently testing the method on the elastic scattering of hydrogen off helium, as this has an exactly solvable scattering amplitude with which to compare. The results are as yet inconclusive.

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[1] L. I. Schiff, Phys. Rev. **103**, 443 (1956).