

Quantum dynamics of large systems - challenges and possible solutions

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Quantum dynamics is ubiquitous in chemistry; it underlies photochemistry, electron transfer processes, non-radiative transitions, spectroscopy and much more. However, elucidating the quantum dynamics of complex systems remains a central challenge.

The problem has two aspects to it. One is the cost of solution of the time dependent Schrödinger equation which typically grows exponentially with the dimensionality of the system. Not less problematic is the fact that quantum dynamics is nonlocal in general and depends on the global potential surface which is rather difficult to generate, for systems with many degrees of freedom. In this talk I will review the main methodologies available for solution of the quantum dynamics and the promise of further progress based on the use of on-the-fly semiclassical methods.

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