Simulating quantum dynamics: first steps towards more efficient Monte Carlo methods
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Although quantum mechanics has an essential probabilistic interpretation, devising stochastic methods for solving large quantum mechanical problems has proven challenging. The challenge is especially difficult for simulating the non-equilibrium behavior of quantum systems. I will describe a master equation for quantum Markovian non-equilibrium dynamics and the wavefunction Monte Carlo method that solves this equation. Deterministically, the cost in solving the master equation scales as N-squared, while stochastically the cost in using the wave function method scales as N. N is the size of the Hilbert space for the problem at hand. Unfortunately, N scales exponentially with the physical size of system under consideration, severely limiting the use of the current wave function Monte Carlo method. Breaking this curse of dimensionality appears to need Monte Carlo methods that sample from complex-valued functions. I will discuss some designs for doing this. The intent of the presentation is to acquaint others with this challenging and important problem. I will give background for key quantum mechanical concepts.