Iterative Monte Carlo in Real-Time Dynamics

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We use the iterative Monte Carlo (IMC) method to calculate the autocorrelation functions of quantum systems. We course-grain sample grid points on a multidimensional lattice with Metropolis Monte Carlo using the imaginary time path integral representation of the Boltzmann density matrix as the sampling function, and propagate the integrand in time at fixed intervals using iterative matrix-vector multiplication. To improve convergence, we introduce filtering factors based on semiclassical and forward-backward approximations, which eliminate the most severe phase cancellation associated with heavier atoms and/or high temperature calculations.