Iterative Monte Carlo Path Integral Formulation of Quantum Dynamics

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An iterative Monte Carlo (IMC) formulation of discretized path integral expressions is presented. This method constitutes a stepwise propagation on a grid selected by a Metropolis Monte Carlo random walk. The use of a spatial configurations selected by a Monte Carlo procedure makes IMC a viable methodology for calculations in polyatomic systems. For equilibrium calculations, IMC is completely equivalent to the standard path integral Monte Carlo (PIMC) method. However, for dynamical (real- or complex-time) calculations, the stepwise evaluation of the discretized path integral implemented in IMC leads to exponential reduction of statistical error compared to a PIMC calculation with the same computational effort. Because IMC circumvents the exponential growth of statistical error with increasing propagation time, it allows stable propagation over long time intervals. The IMC formulation of real- and complex-time correlation functions will be described. Numerical results on multidimensional model systems over propagation up to 30 times the "thermal" time $\hbar\beta/2$ illustrate the capabilities of the method.