Quantum Monte Carlo tunneling from quantum chemistry to quantum annealing

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Quantum Tunneling is important not only for describing quantum chemical reactions, but also quantum computers. Quantum annealers (QA) are a special kind of quantum computers, which make use of quantum fluctuations to escape local minima of the energy landscape in the search for a solution of a combinatorial optimization problem.[1] Here, quantum tunneling could provide a large advantage, compared to classical optimization methods, such as simulated annealing, in particular when the optimization energy landscape displays tall but thin barriers.[2]

In general, to assess the performance of a real QA one should simulate the real-time quantum dynamics. This task is unfeasible for high-dimensional systems, however quantum tunneling also shows up in path integral quantum Monte Carlo (PIMC) simulations. Although PIMC techniques are rigorously derived to describe equilibrium properties, we show that equilibrium PIMC simulations also provide important dynamical quantities. We find that the PIMC tunneling rate displays the same scaling with system size, as the rate of incoherent tunneling. The scaling in both cases is $\mathcal{O}(\Delta^2)$, where Δ is the tunneling splitting (or equivalently the minimum spectral gap). An important consequence is that QMC simulations can be used to predict the performance of a QA for tunneling through a barrier. Moreover, by using open instead of periodic boundary conditions in imaginary time, we obtain a quadratic speedup for PIMC simulations, and achieve linear scaling in Δ. We numerically demonstrate this property over a wide range of problem classes, from spin systems[3] to continuos variables models for proton transfer reactions.[4] We provide a physical understanding of these results due to the existence of an instanton path, which always connects the reactant state with the product.

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