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Diffusion of topological charge and scaling of autocorrelation times in hybrid Monte Carlo simulations of lattice QCD

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We determine the scaling behavior of the autocorrelation times of observables constructed from the topological charge density on lattices with periodic and open boundary conditions using a series of high-statistics numerical simulations. The autocorrelation functions of such observables turn out to obey a simple differential equation which allows the motion of topological charge in hybrid Monte Carlo simulations to be understood in terms of only two processes: diffusion and tunneling. There is a characteristic lattice spacing at which open boundary conditions become worthwhile for reducing autocorrelations and we show how this lattice spacing is related to the diffusion constant, the tunneling rate, and the lattice Euclidean time extent.

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