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Instantons and scaling of the transitions rates in Quantum Monte Carlo simulations of thermally-assisted quantum tunneling in spin systems[1] VADIM SMELYANSKIY, Google, ZHANG JIANG, Stinger Ghaffarian Technologies, Inc., SERGIO BOIXO, SERGEI ISSAKOV, Google, GUGLIELMO MAZZOLA, MATTHIAS TROYER, Swiss Federal Institute of Technology in Zurich, HARTMUT NEVEN, Google — We study analytically and numerically the dynamics of the quantum Monte Carlo (QMC) algorithm to simulate thermally-assisted tunneling in mean-field spin models without conservation of total spin. We use Kramers escape rate theory to calculate the scaling of the QMC time with the problem size to simulate the tunneling transitions. We develop path-integral instanton approach in coherent state and Suzuki-Trotter representations to calculate the escape rate and most probable escape path in QMC dynamics. Analtytical results are in a good agreement with numerical studies. We identify the class of models where the exponent in the scaling of the QMC time is the same as that in physical tunneling but the pre-factor depends very significantly on the QMC path representation. We propose the classes of problems where QMC can fail to simulate tunneling efficiently.

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