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Applications of the worldline Monte Carlo formalism in quantum mechanics. (English)

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Summary: In recent years efficient algorithms have been developed for the numerical computation of relativistic single-particle path integrals in quantum field theory. Here, we adapt this "worldline Monte Carlo" approach to the standard problem of the numerical approximation of the non-relativistic path integral, resulting in a formalism whose characteristic feature is the fast, non-recursive generation of an ensemble of trajectories that is independent of the potential, and is thus universally applicable. The numerical implementation discretises the trajectories with respect to their time parametrisation but maintains a continuous spatial domain. In the case of singular potentials, the discretised action gets adapted to the singularity through a "smoothing" procedure. We show for a variety of examples (the harmonic oscillator in various dimensions, the modified Pöschl-Teller potential, delta-function potentials, the Coulomb and Yukawa potentials) that the method allows one to obtain fast and reliable estimates for the Euclidean propagator and use them in a certain time window suitable for extracting the ground state energy. Usually Monte Carlo calculations in quantum mechanics are performed using algorithms that involve a more specific adaptation to the potential, and we briefly compare our method with the most widely used such algorithms, which are of Metropolis type. As an aside, we apply it for studying the classical limit where nearly classical trajectories are expected to dominate in the path integral. We expect the advances made here to be useful also in the relativistic case.

MSC:

81S40 Path integrals in quantum mechanics
65C05 Monte Carlo methods

Keywords:

path integral; Monte Carlo simulation; quantum mechanics; ground state energy; Coulomb-like singularity

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