Abstract Submitted
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Path integral Monte Carlo on a lattice II: bound states[1] MARK O'CALLAGHAN, BRUCE MILLER, Texas Christian University — The equilibrium properties of a single quantum particle (qp) interacting with a classical gas for a wide range of temperatures that explore the system's behavior in the classical as well as in the quantum regime is investigated. Both the qp and atoms are restricted to sites on a one-dimensional lattice. A path integral formalism developed within the context of the canonical ensemble is utilized, where the qp is represented by a closed, variable-step random walk on the lattice. Monte Carlo methods are employed to determine the system's properties. To test the usefulness of the path integral formalism, the Metropolis algorithm is employed to determine the equilibrium properties of the qp in the context of a square well potential, forcing the qp to occupy bound states. We consider a one-dimensional square well potential where all atoms on the lattice are occupied with one atom with an on-site potential except for a contiguous set of sites of various lengths centered at the middle of the lattice. Comparison of the potential energy, total energy, the energy fluctuations and the correlation function are made between the results of the Monte Carlo simulations and the analytical calculations.

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