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Equilibrium Properties of a Particle Hopping on a Lattice: A Path Integral Study MARK O'CALLAGHAN, BRUCE MILLER, Texas Christian University — We study the equilibrium properties of a single quantum particle (qp) hopping on a one-dimensional lattice. We develop the path-integral formalism in which the quantum particle is represented by a closed variable-step random walk on the lattice. Here we explicitly consider the case of a free particle, which can be directly compared with an analytical solution. We utilize the canonical ensemble and derive expressions for the energy, it's mean square fluctuation, and the qp-qp correlation function in position. One interesting and salient feature of the computation algorithm that shall be stressed is the importance of computing the bins for the probability of a step of a certain size and direction from least probable to most probable, since in this way additions will be performed from very small numbers progressively to larger numbers. If care is not taken in this manner, errant numerical artifacts are introduced simply because of the error associated with addition (subtraction) of very small numbers to (from) much larger numbers. The intention of this paper is to review the derivations of the aforementioned and provide evidence from numerical (Monte Carlo) simulation of the benefits of the algorithm.

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