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Efficiency of rejection free Monte Carlo methods HIROSHI WATANABE, Department of Complex, Systems Science, Graduate School of Information Science, Nagoya University, YUKAWA SATOSHI, Department of Applied Physics, School of Engineering, The University of Tokyo, MARK A. NOVOTNY, Department of Physics & Astronomy, ERC Center for Computational Sciences, Mississippi State University, NOBUYASU ITO, Department of Applied Physics, School of Engineering, The University of Tokyo — We construct asymptotic arguments for the waiting time, the number of trials to achieve one update in Monte Carlo (MC) methods. We find that the waiting time is proportional to e^{β} in the Ising, $\sqrt{\beta}$ in the classical XY, and β in the classical Heisenberg spin systems with inverse temperature β, regardless of the dimension. The behavior in hard particle systems is also obtained, and found to be proportional to $(\rho c - \rho)^{-d}$ with the closest packing density ρc, density ρ, and dimension d of the systems. The waiting time determines the efficiency of rejection-free Monte Carlo (RFMC) methods, as well as the inefficiency of the standard MC. Our arguments are general, and applicable to any RFMC implementation of any model studied using kinetic Monte Carlo.

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