Validity of Molecular Dynamics Simulations for Soft Matter

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In this work, we analytically examine the validity of molecular dynamics for a soft potential system by considering a simple one-dimensional system with a piecewise continuous linear repulsive potential wall having a constant slope a. We derive an explicit analytical expression for an inevitable relative energy change ΔE due to the discreteness, which is dependent on just two parameters: 1) α, which is a fraction of time step τ immediately after the collision with the potential wall, and 2) $\mu \equiv \frac{a\tau}{p_0}$, where p_0 is the momentum immediately before the collision. The whole space made by the two parameters α and μ can be divided into an infinite number of regions, where each region creates a positive or negative energy change ΔE. On the boundaries of these regions, energy does not change, *i.e*, $\Delta E = 0$. The maximal envelope of $|\Delta E|$ *vs.* μ shows a power law behavior $|\Delta E| \propto \mu^{\beta}$, with the exponent $\beta \approx 0.95$. This implies that the round-off error in energy introduced by the discreteness is nearly proportional to the discrete time step τ.