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Jamming and free energy landscapes for three caged soft disks

XIN DU, Graduate student, ERIC WEEKS, Professor — We use a Monte Carlo simulation to study jamming in a model of three soft Brownian disks with harmonic repulsive potential confined in a circular corral. For large corrals, the disks can freely rearrange where one particle passes in between the other two, but for small corrals rearrangements become rare. Rearrangement events correspond to the system crossing over the energy barrier. With low temperature and/or small corral size, the energy barrier becomes larger and the system approaches a glass transition. We calculate the Helmholtz free energy from the distribution of configurations in the system and quantify both the entropic and potential components of the free energy barrier. In a hard disk model, the free energy barrier for rearrangements is entirely entropic. By comparing the entropic component of the soft model to a model of hard disks, we model the soft disks as hard disks with a temperature-dependent effective size. We find that our results are generalizable to other soft disk potentials as well.

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None

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