Computational methods for optimizing interparticle interactions using inverse methods

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We formulate statistical-mechanical inverse methods in order to determine optimized interparticle interactions that spontaneously produce target many-particle configurations. Motivated by advances that give experimentalists greater and greater control over colloidal interaction potentials, we propose and discuss two computational algorithms that search for optimal potentials for self-assembly of a given target configuration. The first optimizes the potential near the ground state and the second near the melting point. We begin by applying these techniques to assembling open structures in two dimensions (square and honeycomb lattices) using only circularly symmetric pair interaction potentials; we demonstrate that the algorithms do indeed cause self-assembly of the target lattice. Our approach is distinguished from previous work in that we consider (i) lattice sums, (ii) mechanical stability (phonon spectra), and (iii) annealed Monte Carlo simulations. We also devise circularly symmetric potentials that yield chain-like structures as well as systems of clusters.