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Ground-State Properties and Phase Separation of Binary Mixtures in Nonscopic Ring Lattices

Authors: Vittorio Penna, Alessandra Contestabile and Andrea Richaud

Abstract: We investigated the spatial phase separation of the two-components forming a bosonic mixture distributed in four well sites in a ring geometry. We studied the ground state of this system, described by means of a binary Bose–Hubbard Hamiltonian, by implementing a well-known coherent-state picture which allowed us to find the semi-classical equations determining the distribution of boson components in the ring lattice. Their fully analytic solutions, in the limit of large boson numbers, provide the boson populations at each well as a function of the interspecies interaction and of other significant model parameters, while allowing to reconstruct the non-trivial architecture of the ground-state four-well phase diagram. The comparison with the i=2,3,4 phase diagram highlights how increasing the number of wells considerably modifies the phase diagram structure and the transition mechanism from the full-demixing phase controlled by the interspecies interaction. Despite the fact that the phase diagrams for i=2,3,4 share various general properties, we show that, unlike attractive binary mixtures, repulsive mixtures do not feature a transition mechanism which can be extended to an arbitrary lattice size l.

Functional Dynamics of Substrate Recognition in TEM Beta-Lactamase

Authors: Chris Avery, Lonnie Baker and Donald J. Jacob

Abstract: The beta-lactamase enzyme provides effective resistance to beta-lactam antibiotics due to substrate recognition controlled by point mutations. Recently, extended-spectrum and inhibitor-resistant mutants have become a global health problem. Here, the functional dynamics that control substrate recognition in TEM beta-lactamase are investigated using all-atom molecular dynamics simulations. Comparisons are made between wild-type TEM-1 and TEM-2 and the extended-spectrum mutants TEM-10 and TEM-52, both in apo form and in complex with four different antibiotics (ampicillin, amoxicillin, cefotaxime and ceftazidime). Dynamic allostery is predicted based on a quasi-harmonic normal-mode analysis using a perturbation scan. An allosteric mechanism known to inhibit enzymatic function in TEM beta-lactamase is identified, along with other allosteric binding targets. Mechanisms for substrate recognition are elucidated using multivariate comparative analysis of molecular dynamics trajectories resulting from changes in dynamics resulting from point mutations and ligand binding, and the conserved dynamics, which are functionally important, are extracted as well. The results suggest that the H9-H10 loop (residues 194-202) is distal from the active site and stabilizes the protein against structural changes. These secondary non-catalytically-active loops offer attractive targets for novel noncompetitive inhibitors of TEM beta-lactamase.

Kinetic Theory and Memory Effects of Homogeneous Inelastic Granular Gases under Nonlinear Drag

Authors: Alberto Moggi and Amb изменения

Abstract: We study a dilute granular gas emmersed in a thermal bath made of smaller particles. The mass is not much smaller than the granular ones in this work. Granular particles are assumed to have inelastic and hard interactions, losing energy in collisions as accounted by a constant coefficient of normal restitution. The interaction with the thermal bath is modeled by a nonlinear drag force plus a white-noise stochastic force. The kinetic theory for this system is described by an Eikok-Fokker-Plack equation for the one-particle velocity distribution function. To get explicit results of the temperature, density and steady states, Maxwellian and first Sonine approximations are developed. The latter takes into account the coupling of the excess kurtosis with the temperature. Theoretical predictions are compared with direct simulation Monte Carlo and event-driven molecular dynamics simulations. While good results for the temperature and steady states are obtained from the Maxwellian approximation, a much better agreement, especially as inelasticity and drag nonlinearity increase, is found when using the first Sonine approximation. The latter approximation is, additionally, crucial to account for memory effects such as alfombra and other phenomena.