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Section Information:

The statistical physics section, broad and interdisciplinary in scope, intends to focus on the challenges of modern statistical physics and its applications to borderline problems while incorporating a high degree of mathematical rigor. Its aim is to provide a collection of high-quality research papers that meet the interest not only of physicists working in this field but also mathematicians and engineers interested in interdisciplinary topics. Generally, papers in pure statistics will not be accepted.

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Section Statistical Physics

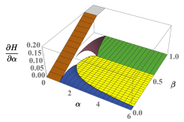
Featured Papers

DOI:10.3390/e23070821

Ground-State Properties and Phase Separation of Binary Mixtures in Mesoscopic 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 a four-well lattice with 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 L-well (L=2,3) phase diagrams highlights how increasing the number of wells considerably modifies the phase diagram structure and the transition mechanism from the full-mixing to the full-demixing phase controlled by the interspecies interaction. Despite the fact that the phase diagrams for L=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 of size L.

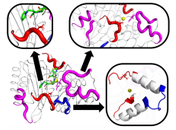


DOI:10.3390/e24050729

Functional Dynamics of Substrate Recognition in TEM Beta-Lactamase

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

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 to identify 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 H10-H11 loop (residues 214-221) is a secondary anchor for larger extended spectrum ligands, while 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.



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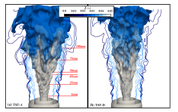
DOI:10.3390/e24050615

Computation of Entropy Production in Stratified Flames Based on Chemistry Tabulation and an Eulerian Transported Probability Density Function Approach

Authors: Louis Dressler, Hendrik Nicolai, Senda Agrebi, Florian Ries and Amsini Sadiki

Abstract: This contribution presents a straightforward strategy to investigate the entropy production in stratified premixed flames. The modeling approach is grounded on a chemistry tabulation strategy, large eddy simulation, and the Eulerian stochastic field method. This enables a combination of a detailed representation of the chemistry with an advanced model for the turbulence chemistry interaction, which is crucial to compute the various sources of exergy losses in combustion systems. First, using detailed reaction kinetic reference simulations in a simplified laminar stratified premixed flame, it is demonstrated that the tabulated chemistry is a suitable approach to compute the various sources of irreversibilities. Thereafter, the effects of the operating conditions on the entropy production are investigated. For this purpose, two operating conditions of the Darmstadt stratified burner with varying levels of shear have been considered. The investigations reveal that the contribution to the entropy production through mixing emerging from the chemical reaction is much larger than the one caused by the stratification. Moreover, it is shown that a stronger shear, realized through a larger Reynolds number, yields higher entropy production through heat, mixing and viscous dissipation and reduces the share by chemical reaction to the total entropy generated.



DOI:10.3390/e24101436

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

Authors: Alberto Megías and Andrés Santos

Abstract: We study a dilute granular gas immersed in a thermal bath made of smaller particles with masses 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 Enskog–Fokker–Planck equation for the one-particle velocity distribution function. To get explicit results of the temperature aging 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 granular temperature 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 Mpemba and Kovacs-like ones.