Orientational ordering and correlations in a quasi-one-dimensional hard-dumbbell fluid

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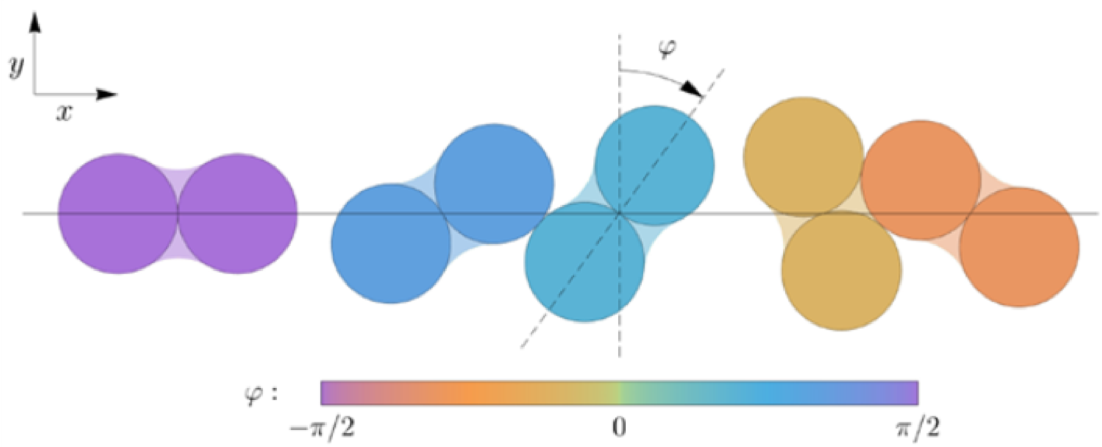
We present an exact theoretical study of a quasi-one-dimensional fluid of anisotropic hard dumbbells with continuous orientational degrees of freedom, which represents a minimal yet nontrivial model that captures the complex interplay between positional and orientational ordering under strong confinement [1]. By formulating the problem within a transfer-matrix framework, we obtain a fully analytical description of the system in terms of the spectral properties of an underlying integral operator. This approach allows us to go beyond approximate or numerical treatments and derive closed-form, exact expressions for key structural and thermodynamic quantities.

In particular, we derive exact results for the equation of state, the orientational distribution function, and both the partial radial distribution functions—defined between particles with specified orientations—and the total radial distribution function—defined between two particles regardless of their orientations. The asymptotic behavior of correlations is determined rigorously through the analytic structure of the Laplace-transformed correlation functions, whose poles, which can be either real or complex conjugates, define the positional and orientational correlation lengths.

Our analysis reveals a rich phenomenology driven by volume-exclusion effects. At intermediate and high densities, we identify an extended regime in which the radial distribution function exhibits an effective algebraic decay over several decades before crossing over to the exponential asymptotic decay dictated by the leading poles. Concurrently, the system undergoes a continuous crossover in orientational ordering, evolving from a weakly ordered, unimodal distribution to a strongly constrained, bimodal state. This structural evolution is accompanied by a nonmonotonic pressure relative to the Tonks gas and by a qualitative transition in correlation decay from oscillatory to monotonic behavior.

In the high-pressure limit, near the close-packing density, we show analytically that positional and orientational fluctuations contribute equally to the pressure, yielding a universal result in which the pressure approaches twice that of the Tonks gas.

Our results are corroborated by numerical solutions of the discretized transfer operator and supported by scaling arguments that rationalize the emergence of the observed regimes. Beyond providing a rare example of an interacting fluid model with exact, closed-form solutions for both structure and thermodynamics, this work establishes a benchmark for testing approximations and offers new insight into ordering phenomena in confined anisotropic systems.



[1] A. M. Montero, P. Gurin, S. Varga, and A. Santos, "Orientational ordering and correlations in a quasi-one-dimensional fluid of hard dumbbells," Phys. Rev. E (accepted 1 April 2026), doi:10.1103/sdt7-t224.