Structural properties of hard-disk fluids under single-file confinement

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We consider a fluid of hard disks of unit diameter confined between two parallel walls separated by a distance $w = 1 + \epsilon \leq 1 + \sqrt{3}/2$ such that each disk can only interact with its two nearest neighbors. This highly confined system can be treated as a quasi one-dimensional (Q1D) system, where its longitudinal properties can be studied from an exact statistical-mechanical perspective.

In this work, we study the structural properties by means of a mapping of the original system onto a one-dimensional polydisperse mixture of non-additive hard rods [1], with all species in the mixture having equal chemical potential. The main idea of this mapping is that the transverse coordinate of each disk, $-\epsilon/2 < y < \epsilon/2$ represents the dispersity parameter and the longitudinal separation at contact, $a(y - y') = \sqrt{1 - (y - y')^2}$ is the hard-core distance of two 'species' (y and y'). A schematic representation of this mapping is shown in Fig. 1.

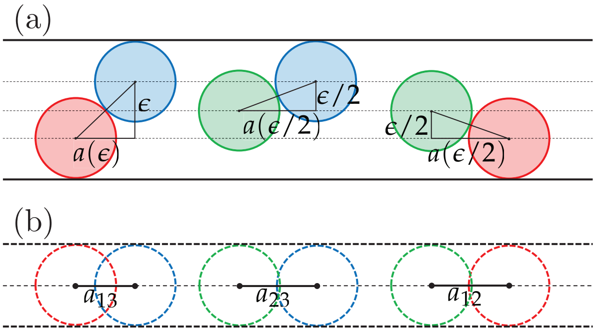

Fig. 1. Schematic representation of the mapping of (a) the original Q1D system onto (b) a 1D mixture of non-additive hard rods.

Standard liquid theory of mixtures is then used as a starting point to derive exact thermodynamic and structural properties, such as the structure factor, the radial distribution function (RDF) or the correlation length, of the mapped one-dimensional system. Comparisons with Monte Carlo simulation methods performed in the original Q1D system show an excellent agreement in all studied quantities. Figure 2 shows the longitudinal RDF for several values of the linear density λ for the maximum possible value of the channel width.

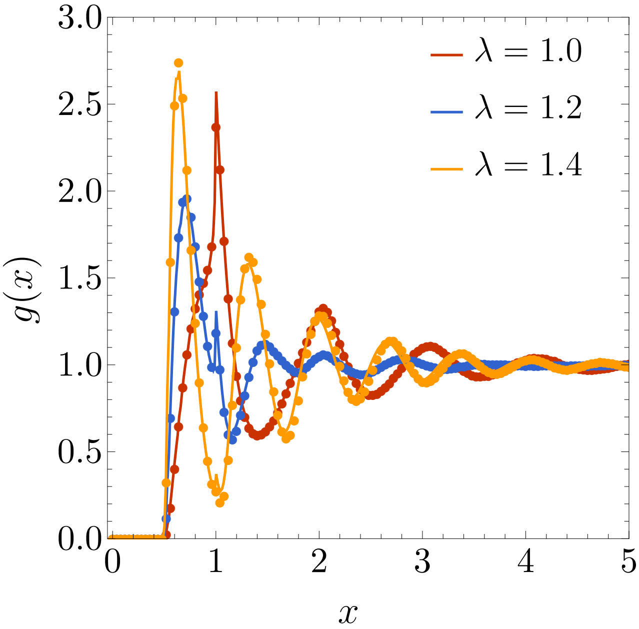

Fig. 2. RDF $g(x)$ for different values of density at $\epsilon = \sqrt{3}/2$. Solid lines are out theoretical results, while symbols are MC data from Ref. [2].

We have also analyzed the scaling form of the disappearance of defects in the zigzag configuration at high pressures. Moreover, by studying the nonzero poles of the Laplace transform of the RDF, we have obtained the translational correlation length and the asymptotic oscillation frequency, which show that a *structural crossover* takes place at a certain crossing pressure, where the asymptotic oscillation frequency experiences a discontinuous jump.

[1] A. M. Montero, and A. Santos, *Equation of state of hard-disk fluids under single-file confinement*, J. Chem. Phys. **158**, 154501 (2023).

[2] S. Varga, G. Balló, and P. Gurin, *Structural properties of hard disks in a narrow tube*, J. Stat. Mech. **2011**, 11006 (2011).