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ELASTIC PROPERTIES OF SOFT DISK CRYSTALS

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Abstract. The influence of potential softness on the elastic properties of soft disks, interacting through *n*-inverse-power potentials, r^{-n}, has been investigated in a Monte Carlo simulation. Two mechanisms influencing Poisson's ratio have been revealed: (*i*) particle motions decrease the ratio at high densities with respect to the static (zero temperature) case and (*ii*) the ratio can be also decreased at fixed temperatures and pressures by increasing *n*. Simulations have shown that the hard disk's elastic constants can be obtained in the limit $n \to \infty$. When $T \to 0$, the elastic constants of soft disks tend to those of the static model.

1. INTRODUCTION

Investigation of a simple model is the first step in understanding phenomena observable in complex real systems. In recent years, there has been growing interest in studying various physical systems which can be described using their inverse power potential [1–11],

$$u(r) = \epsilon \left(\frac{\sigma}{r}\right)^{n}, \tag{1}$$

where *r* is the distance between the interacting particles, σ is the particle's diameter, ϵ sets the energy scale and *n* is a parameter determining the potential hardness (the softness parameter is defined as its inverse, n^{-1}).

This paper is focused on the elastic properties of soft disk crystals in two dimensions, which have not been investigated yet. The structure of the paper is as follows. Basic details of the simulations are given in Sec. 2. The simulation's results are presented and discussed in Sec. 3. They are compared with a static lattice interacting by the *n*-inverse-power potential in the $n \to \infty$ limit corresponding to hard disks at close packing. They are also compared with a hard disk system at a positive temperature. Sec. 4 contains a summary and conclusions.

2. SIMULATION DETAILS

The simulations were performed in a *NpT* ensemble by the Monte Carlo method, following the Parrinello-Rahman idea of averaging strain fluctuations [12–14]. The applied version of the method was based on Refs. 15,16. The strain expansion of the free enthalpy (Gibbs free energy *G*) of a two-dimensional hexagonal crystal under isotropic pressure is as follows [16]:

$$G = G(0) + \frac{B}{2} V_p (\varepsilon_{xx} + \varepsilon_{yy})^2 + \frac{\mu}{2} V_p (4\varepsilon_{xy}^2 + (\varepsilon_{xx} + \varepsilon_{yy})^2), \tag{2}$$

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where $G(0)$ is the free enthalpy of a system without deformation whose volume is V_p, B is the bulk modulus, μ is the shear modulus, and ε_{ij} are the strain tensor's components.

The Poisson ratio is defined as the negative ratio of transverse strain to longitudinal strain when the stress parallel to the longitudinal direction is changed [17]. In the case of a two-dimensional crystal under pressure it is equal to [6]

$$\nu = \frac{B - \mu}{B + \mu}. \tag{3}$$

All simulations were performed in reduced (dimensionless) units: energy $E^* = E/\epsilon$, density $\rho^*=\rho\sigma^2 \equiv N\sigma^2/V$, temperature $T^* = k_B T/\epsilon$, pressure $p^* = p\sigma^2/\epsilon$, the bulk modulus $B^* = B\sigma^2/\epsilon$, and the shear modulus $\mu^* = \mu\sigma^2/\epsilon$.

Two kinds of trial motions were used. One concerned a change in an individual disk position and its acceptance ratio was kept close to 30 percent. (The 'moving' disks were sequentially selected, as no statistically significant differences were observed between such runs and some trial runs with random selection.) The other corresponded to changes in the components of the (symmetric) box matrix and was tried about $N^{1/2}$ times less frequently than the disk motion. Its acceptance ratio was close to 20 percent.

Most simulations were performed for a system of $N = 224$ particles, with a periodic boundary condition, whose $T = 0$ ground state configuration was a triangular lattice occupying a rectangular (almost square) box $14a_0$ wide (a_0 being the nearest-neighbor distance) and $8\sqrt{3}a_0$ high.

Table 1. Comparison of the bulk and shear moduli of the system with r^{-12} interaction potential obtained in the present work and in [5,7]. Density, pressure and temperature are expressed in reduced units $\rho^*=1.050(1)$, $p^*=17.45$ and $T^*=1$. ∞ in the first column represents extrapolation to $N\to\infty$.

N	B^*	μ^*	Refs.
56	84.8(6)	23.8(4)	present work
224	84.1(7)	24.0(5)	present work
780	83.4(5)	24.4(3)	present work
∞	83.5(6)	24.3(4)	present work
780	83(2)	24.6(6)	Broughton *at al.* [5]
780	78(3)	23.3(7)	Sengupta *at al.* [7]

Other system sizes were also studied to estimate the result's dependence on number of particles, see Table 1.

The typical length of runs for $N = 224$ was equal to $5 \cdot 10^6$ trial steps per particle (cycles) after equilibration. Some longer runs were also performed to analyze the method's convergence and verify the consistency of our results with those of others. In Table 1 the present results are compared with the data available in the literature for the bulk and shear moduli. Very good agreement of our results with those of Broughton *et al.* [5] confirms of the reliability of our calculations. There are some discrepancies between our results and those obtained by Sengupta *et al.* [7]. Its origin is not clear.

3. RESULTS AND DISCUSSION

A. The static limit (T = 0)

The influence of particle motions (i.e. positive temperature) on the elastic properties of a hard disk system in the close packing limit can be ascertained by considering a static, i.e. *zero- temperature*, triangular lattice whose nearest-neighboring sites (distanced by a) interact by potential (1) in the $n\to\infty$ limit, which can be thought of as the hard-potential limit. The pressure, bulk modulus, shear modulus, and Poisson ratio of such a lattice are as follows

$$p^{static} = \sqrt{3}n \in a^{-(n+2)}, \tag{4}$$

$$B^{static} = \frac{n+2}{2} p^{static}, \tag{5}$$

$$\mu^{static} = \frac{n-2}{4} p^{static}, \tag{6}$$

$$\nu^{static} = \frac{n+6}{3n+2}. \tag{7}$$

B. The bulk and shear moduli

For a large enough n, the static model defined in the previous subsection can be thought of as the zero-temperature limit of the model of soft disks interacting through the potential (1) [16].

The dependence of the dimensionless bulk modulus and the shear modulus on the softness parameter, $1/n$, is shown in Figs.1a and 1b for various values of exponent $12 \le n \le 768$ and temperatures in the $0.001 \le T \le 1$ range, under pressure $p^* = 15.4$. In the $n\to\infty$ limit, the elastic modulus reaches values corresponding to those of the hard disk crystal at the given pressure [16].

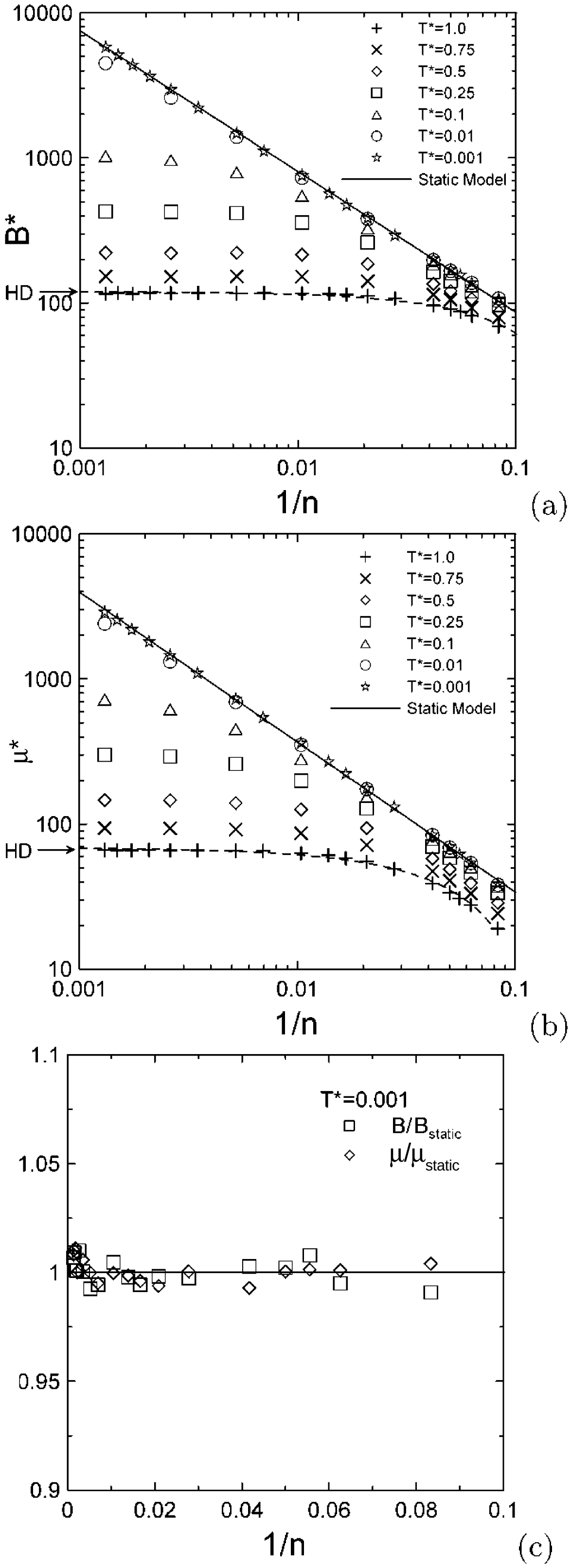

Fig. 1. The (a) bulk and the (b) shear moduli, and (c) rescaled bulk and shear moduli versus the softness parameter n^{-1}, under constant pressure p^* = 15.4.

At the same time, it is apparent from Figs.1a and 1b that the soft disk results at T^* = 0.001 are very close to the static case described by (5)-(6), a conclusion supported by Fig. 1c.

C. The hard disk limit

The temperature dependences of the bulk and shear moduli are presented in Fig. 2 for various n at T^* = 1. Taking T^* = 1.0 and $n \to \infty$, the so-called hard disk limit is obtained. It is easily noticeable in Fig. 2 that, in the hard disk limit, both bulk and shear moduli of soft disks tend to those of hard disks.

D. Poisson's ratio

In Fig. 3a, the Poisson ratio of soft disk systems at the same pressure is plotted versus softness 1/n.

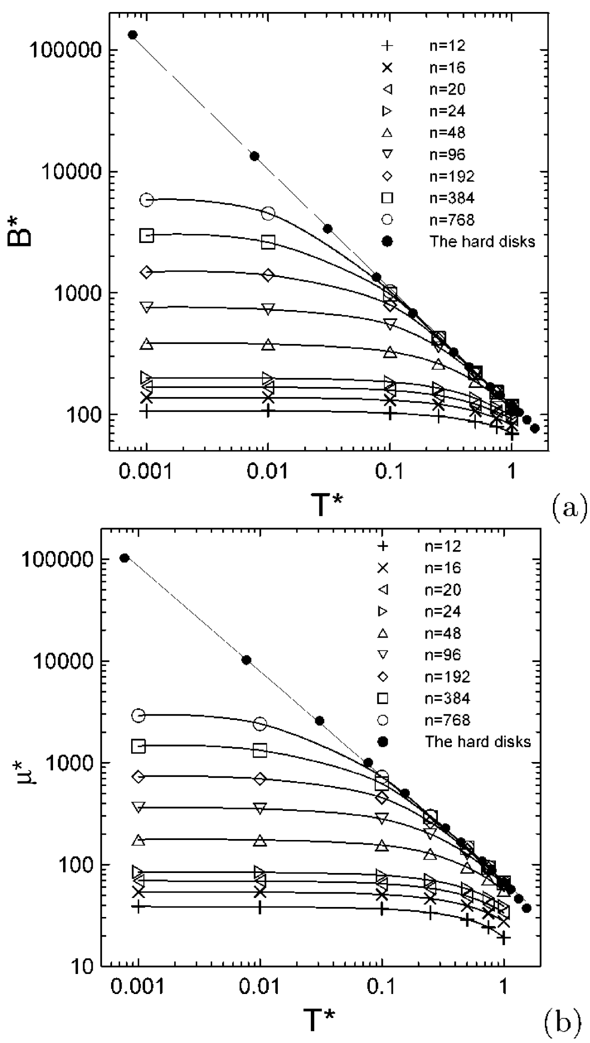

Fig. 2. Temperature dependence of: (a) the bulk modulus and (b) the shear modulus under pressure p^* = 15:4. The solid circles represent the results of the hard disk system from [16]. The lines are drawn to guide the reader's eye.

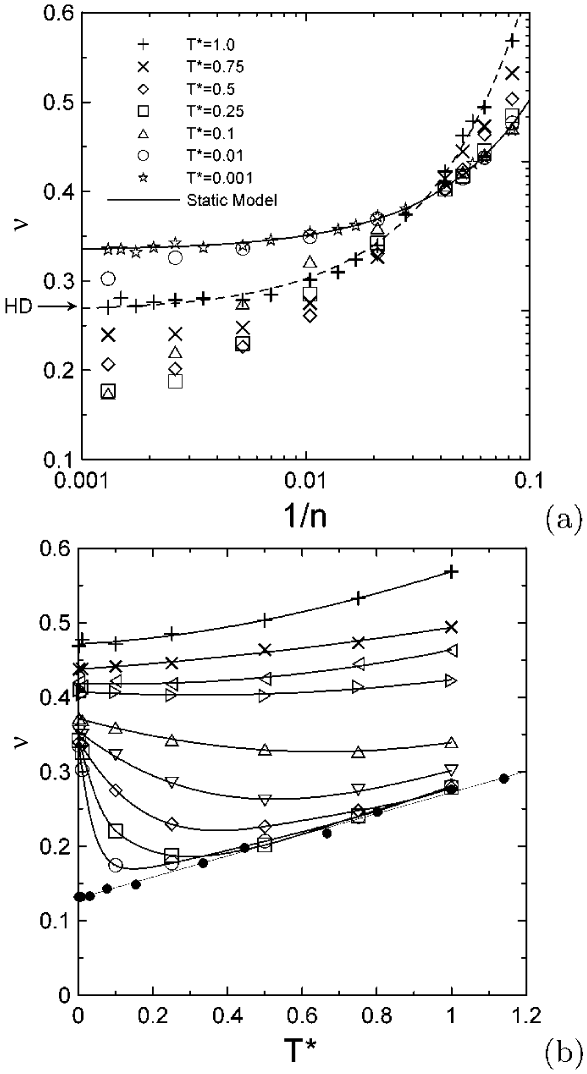

Fig. 3. Poisson's ratio versus: (a) softness and (b) temperature at p^* = 15.4; symbols are the same as in Fig.2. The solid circles in (b) represent results obtained for the hard disk system described in [16]. The dashed line in (a) is drawn for the T^* = 1:0 data to guide the reader's eye. The solid lines in (b) are drawn for the same purpose.

As expected, the limiting value for $n \to \infty$ tends to the Poisson ratio of the hard disk system. In the case when $T^* \to 0$ the values of Poisson's ratio verge towards those of the static model. It is worth noting that for large n and $0.1 \le T^* \le 0.75$ the values of Poisson's ratio are less than for the limiting cases, i.e. the static model and the hard disk system.

Interestingly, particle motions decrease the Poisson ratio of soft disks with respect to the static case (i.e. the zero temperature case) for $n \ge 30$. For $n \le 30$ (cf. the solid and dashed lines in Fig. 3a), the presence of particle motions ($T > 0$) increase Poisson's ratio with respect to the static case ($T = 0$).

The temperature dependence of Poisson's ratio is shown in Fig. 3b. It follows from its analysis that increased power n (i.e. the hardness parameter) in the interaction potential leads to a decrease in Poisson's ratio for soft disks throughout the considered temperature range. At high temperatures and large values of the hardness parameter, Poisson's ratio approaches the hard disk results.

A discontinuity (or "jump") in the Poisson ratio is noticeable in Fig.3b in the $T \to 0$ limit: for very large (but finite) values of the hardness parameter, n, Poisson's ratio tends to 1/3 whereas when $n \to \infty$ the ratio tends to its hard disk limit at close packing, $\nu_{HD} \approx 0.13$ [16]. More discussion of this discontinuity will be presented elsewhere.

Some plots of the Poisson ratio obtained at T^* = 1 are shown in Fig. 4 as a function of the softness parameter for a few pressures. In the $n \to \infty$ limit the values of the Poisson ratio of hard disks [16] are reproduced well. Pressure has a much weaker influence on Poisson's ratio for very soft particles (small n) than for large n.

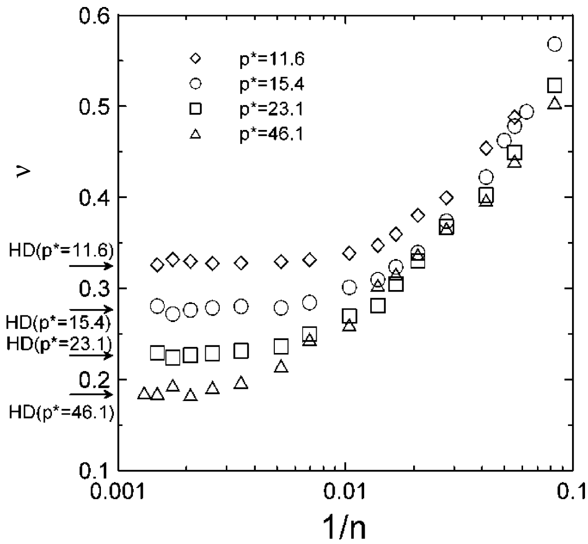

Fig. 4. Poisson's ratio versus the softness parameter at temperature T^* = 1.0, under various pressures. The arrows on the left indicate the hard disk values [16].

4. SUMMARY AND CONCLUSIONS

The elastic properties of a soft disk system have been determined by analysis of the box matrix evolution in Monte Carlo simulations. The static model of hard disks, in which only the nearest neighbors can interact, can be thought of as the low-temperature limit of the soft disk model with the *n*-inverse-power potential when *n* is large. Simulations of soft disks indicate that at $T = 0.001$ the difference between the elastic modulus for that model and that for the static model is less than two percent when $n \geq 12$. At the same time, simulations of soft disks at $T^* = 1$ suggest that the elastic constants of hard disks differ by less than two percent from those of soft disks when $n \geq 192$. Recently, it has been demonstrated that the static model works as well in the three-dimensional case [18].

Particle motions reduce the Poisson ratio of a soft disk system with respect to the static case (i.e. the zerotemperature case) for large *n*. The opposite behavior (i.e. increasing the Poisson ratio by introducing particle motions) is observed when *n* is small.

It has been shown that at a fixed temperature and pressure, the Poisson ratio of a soft disk crystal decreases with increasing hardness parameter *n* for all values of *n* studied.

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