A new solution to the statistics of hard elongated objects

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We propose an analytical solution to the statistics of hard elongated objects (e.g. needles, rectangles, ellipses, etc) in one dimension, by using Gibbs free energy formalism and an adequate approximation to the phase space. Some analytical formulation for a collective thermodynamic properties are found that are in agreements with the results recently obtained numerically from the exact model. We also verify the inverse distance law of sound pressure and notice below a certain pressure the expectation value of inverse distance is deviated from scaling as the inverse of distance.

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I. INTRODUCTION

Elasticity theory describes how a system under distortion is mechanically deformed. There are two approaches to quantitatively study this. The traditional approach is to analyze the dislocation of fluid rigid boundaries. Depending on the properties of fluid (e.g. viscosity, compressibility, etc.) a variety of different cases appears, (see [1]). The other approach, which is of our interest, replaces fluid with discrete objects and studies the short-range interaction between these objects. If the objects are spherically-symmetric, their alignments lead to translational ordered/disordered phases, [2, 3, 4]. Frenkel et.al. in a series of papers (see [5]) developed a method that enables to analyze the stress and elasticity of hard spherically-symmetric objects.

A natural generalization is to replace the spherically-symmetric objects with elongated objects. These objects carry a coupling between their translational and rotational degrees of freedom and display orientational ordered/disordered phases; similar to liquid crystals [6]. Recently, in a series of papers a formalism for direct calculation of elastic properties of hard non-spherically symmetric objects was proposed by Murat, Kantor, and Farago (see [7]). They considered hard stiffness for these objects in order to prevent the influence of orientational degrees of freedom into kinetic energy. Their method was developed on the basis of different types of central and non-central short-range interactions; central potential depends only on the relative distance between particles, whereas noncentral potential depends on individual object orientations. This formalism has been so far applied in different problems such as the wrapping of proteins in DNA [8], the ordering of complex liquids systems and percolation transitions [9], and the jamming transitions, [10]. However, this formalism is hard to be solved analytically and a Monte-Carlo simulation should been used to extract its physical properties. Kantor and Kardar in [11] proposed a self-consistency check for this formalism in one dimension, where instead of non-spherically symmetric objects, needles are applied. The center of needles are on a line and the angle of each needle orientation is randomly chosen. They solved this model by transfer matrix method numerically and reported an agreement between the numerical and MC results.

The purpose of our communication is to reconsider elongated objects in one dimension and propose an analytical solution that, in our opinion, goes a step forward since it allows to obtain analytical formulation for some collective properties obtained so far only numerically. To this end, we eliminate the dependence of free energy on the absolute value of an angle, thus make the orientation completely isotropic. Interparticle distance and elasticity coefficients are derived into analytical formulations and verify the exact model results of [11]. We generalize our formalism to cover different types of elongated objects and repeat to derive them and verify recent results of [11, 12]. This formalism allows to evaluate other properties of the same class, such as inverse distance between needles. We verify the inverse distance law of sound pressure (e.g [14]) in high densities. As expected from a previous study on spherically-symmetric object (see [13]), in needles model the expectation value of inverse distance below a critical pressure does not scale as the inverse of distance.

FIG. 1: The phase space diagram of needles model.

In needles model, a number of needles with centers located on a straight line are considered. Each needle has two degrees of freedom: translational \( x \), and rota-
tional $\phi$ (where $-\pi/2 \leq \phi \leq \pi/2$). When two needles touch one another their orientations displays their minimum distance. This distance is $\ell_X_{i,i+1}$ with $X_{i,i+1} = \sin(|\phi_i - \phi_{i+1}|) / \max(\cos(\phi_i, \phi_{i+1}))$, and $\ell$ is a length scale.

The phase space diagram $(X, \phi_1, \phi_2)$ of needles model is depicted in Figure (1). The two maxima at the opposite tips of left and right ‘wings’ denotes the configurations where two adjacent needles are bending tangentially at the central axis. The minima of $X = 0$ denote all different configurations in which two adjacent needles are oriented parallel, $\phi_1 = \phi_2$. Every contour line in Figure (1) denotes a set of degenerate configurations of a corresponding distance. The larger a distance is, the lower its degeneracy becomes.

Following Takanashi’s proposal (see [3]) for studying free energy of hard objects, two adjacent needles, located at $x_i$ and $x_{i+1}$ interact by a hard potential $U(x_i, x_{i+1})$. This potential is zero for larger distances than the minimal distance $\ell_X_{i,i+1}$, and infinite otherwise.

Consider a chain of $N$ needles compressed by the external pressure $p$. By definition the Gibbs free energy is $G = E - TS + PV$. In the lack of temperature dependence, a configuration partition function is defined as $Z_G = \sum e^{-\beta G}$. We assume the kinetic energy of particles is negligible, which means we study the system after all needles are at rest. Hard potential contributes to the partition function: $Z_G = \prod_{i=1}^N \int dx_i \int dx_{i+1} \exp(-\beta (U(x_i, x_{i+1}) + p(x_i - x_{i+1}))).$

Renaming $s_i := |x_i - x_{i+1}|$ and applying hard potential makes up $Z_G = \prod_{i=1}^N \int \phi_i f_{X}^\infty ds_i \exp(-\beta p s_i) = (\beta p)^{-N} \prod_{i=1}^N \int_0^\pi d\phi_i \exp(-\beta p \ell X(\phi_i, \phi_{i+1}))).$ Notice that in thermodynamic limit, open chain and closed chain of needles have the same free energies; (beyond this limit the difference are in a surface free energy that appear in the open chain and scales as 1/N).

In general, two systems behave likewise if their phase spaces are similar. This highlights acceptable approximations that may simplify the free energy associated with the phase space of Figure (1). In the following we consider a phase space in which the wrinkles of Figure (1) are flattened. This is indicated to analytically solve the problem and more importantly it is identical to the original model in the study of some collective properties. We can also easily generalize this formalism to also study some different types of elongation, other than needles.

II. THE FORMALISM

Consider the minimal distance between two particles $i$ and $i+1$ is defined by

$$X_{i,i+1} = \frac{2}{\pi} |\phi_i - \phi_{i+1}|. \quad (1)$$

The corresponding phase space diagram is depicted in Figure (2). Comparing this with Fig. (1) one observes in the latter model the dependence of free energy on single angles has been vanished, therefore orientations are isotropic. We expect the two models behave differently on their ordering at high pressures; however, if we ignore the discussion of ordering and just look at properties such as stress and elasticity coefficients the models behave similarly even at high compression.

Let us define the dimensionless pressure $f = \beta p \ell$. Based on (1) the partition function becomes $Z = f^{-N} \left( \int d\phi_1 d\phi_2 e^{-f \frac{\pi}{2} |\phi_1 - \phi_2|} \right)^N$. In two adjacent particles the angles are independent and each one takes a value between $-\pi/2$ and $\pi/2$. Therefore, using Eq. (1), two needles have the distance $2x$, where $0 \leq x \leq 1$. A two-body partition function becomes

$$Z_1 = f^{-1} \left( \int_0^1 dx e^{-2fx} \right) = \frac{1 - e^{-2f}}{2f^2}. \quad (2)$$

Since the distance between a pair of particles is an independent parameter, the partition function of $N$ particles is $Z = Z_1^N$ and the Gibbs free energy per particles becomes

$$\frac{\beta G}{N} = -\ln Z_1 = 2 \ln f - \ln(1 - e^{-2f}). \quad (3)$$

The first term indicates the orientationally-independent free energy (point particle part) and the second term reflects hard interaction between the particles. The behavior of this free energy in different pressures is plotted in Figure (3) denoted in solid line, and was compared to the point particle behavior in dashed line. This result is in good agreement with the numerical results of Figure (3) in [11] where the full anisotropic model was applied. The analogy of results highlights that the free energy of exact model of [11] is unaffected if its anisotropy is eliminated. In other words, the major contribution into the elasticity of needles in thermodynamic limit is rooted at isotropic features. Consequently, this is not unrealistic to expect the parameters extracted from this free energy behave similar to the original model.

Following the formalism originally proposed for spherically-symmetric objects in [4] and extended to the correlation functions of elongated objects in [7], stress
and elasticity coefficient were introduced in one dimensional systems in [11]. Stress indicates mean distance between particles and is defined as $\alpha = \frac{\partial (G/N)}{\partial f}$ in fixed temperature $T$. Substituting the Gibbs energy from Eq. [3] into this definitions, interparticle distance becomes:

$$\frac{a}{\ell} = \frac{2}{f} - \frac{2}{e^{2f} - 1}$$  \hspace{1cm} (4)

The elastic coefficient is also defined by $C = -\frac{\partial^2 (G/N)}{\partial f^2} + p$. Re-scaling the coefficient into $\beta C$ gives it rise to $\frac{a}{\ell} = \frac{2}{f} - \frac{2}{e^{2f} - 1}$. Using the Gibbs energy in Eq. [3] the elastic coefficient becomes:

$$C = \frac{f}{2} \left[ 4 \cosh(2f) - (2f^2 + f + 4) + f \exp(-2f) \right]$$  \hspace{1cm} (5)

The mean distance $a$ and the elasticity coefficient $C$ are plotted in Figure [4] (see the case of $\alpha = 1$). The (blue) line of negative slope denotes $a$ and of positive slope denotes $C$. The dashed lines in the figure correspond to the mean distance and elastic coefficient of point particles, respectively. The behavior of $a$ and $C$ are in good agreement with those extracted by numerical studies in Figure (4) of [11].

III. A GENERALIZATION INTO ELONGATED OBJECTS

Lebowitz in [13] proposes a generalization into Eq. [1] of the following form:

$$X_{i,i+1}(\phi_1, \phi_2) = \left( \frac{2}{\pi} |\phi_i - \phi_{i+1}| \right)^\alpha$$  \hspace{1cm} (6)

Spacial cases are needles with the exponent $\alpha = 1$, and narrow ellipses with $\alpha = 2$. In general, the case of $\alpha < 1$ describes a phase space almost similar to Figure [2] except that its ‘wings’ get bumps upwards that makes it look like $\gamma$-shape. In the case of $\alpha > 1$ the wings are deformed into two valleys and the phase space diagram looks like a $U$-shape.

In general, the partition function per particle becomes

$$Z_{G/N} = \frac{1}{f} \int_0^1 e^{-f(2x)\alpha} \, dx$$

$$= \frac{1}{2\alpha f^{1+\alpha}} \left( \Gamma \left( \frac{1}{\alpha} \right) - \Gamma \left( \frac{1}{\alpha}, 2\alpha f \right) \right), \hspace{1cm} (7)$$

where $\Gamma(a, x) = \int_x^\infty t^{a-1} e^{-t} \, dt$. To get this function, we renamed $y = f(2x)^\alpha$. Using this partition function, the mean distance for different choices of $\alpha$ could be calculated. The mean distance between the objects will become:

$$\frac{a}{\ell} = \frac{1 + 1/\alpha}{f} - 2f^{(2-\alpha)/\alpha - 1} \exp(-2f) \frac{\Gamma(1/\alpha) - \Gamma(1/\alpha, 2f)}{\Gamma(1/\alpha) - \Gamma(1/\alpha, 2f^\alpha)}.$$  \hspace{1cm} (8)

Here we utilized the chain rule $\frac{d\Gamma(a,u(x))}{dx} = \frac{d\Gamma(a,u)}{du} \frac{du}{dx}$, and $\frac{d\Gamma(a,x)}{dx} = -x^{a-1} e^{-x}$. Finding the elasticity coefficient from $a$ is straightforward.

$C$ and $a$ are plotted in the Figure [4] for the exponents $\alpha = 0.2, 0.5, 1, 2, 5$ from top to bottom, respectively.

$C$ and $a$ are plotted in the Figure [4] for the exponents $\alpha = 0.2, 0.5, 1, 2, 5$ from top to bottom, respectively. The mean distance lines are with negative slopes and the elasticity coefficient lines are with positive slopes. The non-interacting results are depicted in dashed lines. These results have already been derived recently by a numerical analysis in [12].

From the agreement between the results of isotropic and anisotropic, one can conclude that distance and elasticity in elongated object system are highly depended onto the isotropic features such that even at high compressions their anisotropic effects are negligible.
IV. INVERSE DISTANCE

Inverse distance rules the scaling of many parameters in physics. For instance, the inverse distance law governs the damping of sound pressure in a medium inversely proportional to distance from sound source, \[14\]. However, in a granular medium (made of frictional balls) there are deviations from this law, where the velocity of sound propagation scales as \(p^n\) with \(n < 1\) not \(p\). \[17\]. We shall analyze this deviation in the case of elongated objects.

We calculate the expectation value of inverse distance directly from the free energy. The expectation value of inverse distance is defined:

\[
\langle a^{-1} \rangle = \frac{\int dx \frac{1}{x a} e^{-f X(x)}}{\int dx e^{-f X(x)}}
\]

The derivative of left side with respect to \(f\) becomes

\[
\frac{d}{df} \langle a^{-1} \rangle = -1 + \langle a^{-1} \rangle a \tag{9}
\]

From Eq. \[9\] one concludes the relation \(\langle a^{-1} \rangle = 1/a\) is only verified in pressure-independent distance models. In other words if \(a\) depends strictly on pressure the inverse distance will no longer be \(1/a\).

In the present model, mean distance depends on pressure. From Eq. \[9\] we should be able to directly calculate the mean inverse distance. Substitute Eq. \[4\] into Eq. \[9\] gives rise to the following differential equation:

\[
\frac{d}{df} \langle a^{-1} \rangle = -1 + \left( \frac{2}{f} - \frac{2}{e^{2f} - 1} \right) \langle a^{-1} \rangle. \tag{10}
\]

This differential equation has a solution of the form \(\langle a^{-1} \rangle = f + \frac{2 f}{e^{2f} - 1} E_1(2f)\), where \(E_1(z) = \int_1^\infty \frac{e^{-t} t}{t^z} dt\) is the exponential integral function. \(E_1(z)\) is known to behave as a negative exponential for large \(f\) and as a logarithm for small \(f\). This is standard to approximate it by one of its bracketing function bounds (e.g. see \[16\]). In our problem, this allows to replace it with \(\frac{1}{2} e^{-2f} \ln(1 + 1/f)\). Consequently, the expectation value of inverse distance becomes:

\[
\langle a^{-1} \rangle = f + \frac{2 f \ln(1 + 1/f)}{e^{2f} - 1}. \tag{11}
\]

In right side of Eq. \[11\] the first term is point particle contribution, (and verifies the inverse distance law \(\langle a^{-1} \rangle \sim f\) in corresponding medium). The second term denotes the effects of elongation. In high pressures this correction is negligible; however, in low pressures the inverse distance is gradually separated from \(f\) and gets a larger values. Below a certain pressure the inverse distance approaches again to \(f\). This transition is better reflected in the behavior of \(\langle a^{-1} \rangle\). This parameter in point particle medium is the constant 2. Elongated objects display a deviation into it in low pressures, which is plotted in the inset of Figure \[5\].

In conclusion, we think to have presented an accurate method to obtain some collective properties of elongated objects completely analytically. To this end, we proposed to eliminate the dependence of free energy onto the absolute value of an angle, and thus make the orientation completely isotropic. This is expected to change the model to behave differently at high pressures, where the original model becomes strongly ordered; but if we disregard the ordering and just look at other properties (such as pressure or elastic constants) the differences are negligible even at high compressions. The simplicity of this formalism allows a better understanding of the statistics of elongated objects. While this formalism can receive applications into more realistic physical systems such as protein wrapping and adsorption in biology, etc., this can also be employed for studying elongated objects in higher dimensions.

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