

INFUENCE OF DISORDER ON THE POISSON'S RATIO OF STATIC SOLIDS IN TWO DIMENSIONS

Krzysztof W. Wojciechowski and Jakub Narojczyk

Institute of Molecular Physics, Polish Academy of Sciences, M. Smoluchowskiego 17, 60-179 Poznań, Poland

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Abstract. Recent results concerning the Poisson's ratio of three simple two-dimensional (2D) models of aperiodic structures are reviewed. The models, which consist of mono-, bi-, and tri-atomic particles interacting through the n -inverse-power-potential between the nearest-neighbouring atoms, were studied at zero temperature by computer simulations. It is shown that the Poisson's ratio increases with increasing disorder in the models.

1. INTRODUCTION

Modern technology requires new materials of special properties. Efficient designing of such materials will be possible when various mechanisms allowing one to control main characteristics of materials will be revealed and well understood. One of ways to reach this goal is by studying simple models in which all the features are well defined and easy to control.

Elastic properties constitute one of most fundamental characteristics of real materials which is crucial for their mechanical applications. Despite such applications are probably as old as the history of human beings, our knowledge of elastic properties of real media is still far from being complete.

Materials for which the Poisson's ratio [1] is negative, known also as auxetic materials [2-7], constitute a simple example illustrating this opinion.

In this paper some recent works done by the present authors [8-10] are briefly reviewed. The review, concerning three model systems which form elastically *isotropic* phases, concentrates on the influence of disorder on the Poisson's ratio.

The structure of the paper is as follows. In Sec. 2 we remind some basic formulae from the elasticity theory of isotropic systems in two dimensions and sketch the computational method used. In Sec. 3 we describe the systems studied and discuss the obtained results concerning the Poisson's ratio. The last section (Section 4) contains the summary and conclusions.

Corresponding author: Krzysztof W. Wojciechowski, e-mail: kww@ifmpan.poznan.pe

2. COMPUTATION OF THE POISSON'S RATIO OF ELASTICALLY ISOTROPIC 2D MODELS

We start this section with a brief description of the elasticity of 2D isotropic systems and then sketch the method we used to compute the Poisson's ratios of the studied models.

2.1. Elasticity of 2D isotropic media

Two-dimensional (2D) crystals exhibiting an effective 3-fold symmetry axis are elastically isotropic for small deformations, what can be easily shown by applying Landau's argument described in his textbook for solids of 6-fold symmetry axis [1]. Thus, elastic properties of such systems can be described with only two elastic constants, the bulk modulus B and the shear modulus μ .

The elastic free energy of a deformed 2D crystal exhibiting 3-fold symmetry axis can be written in the same way as in the case of the 6-fold symmetry axis, i.e. as a function of the strain tensor components and the elastic constants [1]:

$$F = -p(\varepsilon_{xx} + \varepsilon_{yy}) + 2\lambda_{\zeta\eta\xi\eta}(\varepsilon_{xx} + \varepsilon_{yy})^2 + \lambda_{\xi\xi\eta\eta}[(\varepsilon_{xx} + \varepsilon_{yy})^2 - 4\varepsilon_{xy}^2]. \quad (1)$$

The values of the above mentioned elastic constants, $\lambda_{\zeta\eta\xi\eta}$, $\lambda_{\xi\xi\eta\eta}$, and pressure, p , can be obtained by differentiation of the free energy with respect to the strain tensor components, see e.g. [11]

$$\left. \frac{\partial F}{\partial \varepsilon_{xx}} \right|_{\varepsilon=0} = -p, \quad (2)$$

$$\left. \frac{\partial^2 F}{\partial \varepsilon_{xx}^2} \right|_{\varepsilon=0} = 4\lambda_{\zeta\eta\xi\eta} + 2\lambda_{\xi\xi\eta\eta}, \quad (3)$$

$$\left. \frac{\partial^2 F}{\partial \varepsilon_{xx} \partial \varepsilon_{yy}} \right|_{\varepsilon=0} = 4\lambda_{\zeta\eta\xi\eta} - 2\lambda_{\xi\xi\eta\eta}. \quad (4)$$

The bulk modulus, B , and the shear modulus, μ , are directly related, see e.g. [12], to the quantities used in Eq. (1)

$$B = 4\lambda_{\zeta\eta\xi\eta}, \quad (5)$$

$$\mu = 2\lambda_{\xi\xi\eta\eta} - p. \quad (6)$$

The Poisson's ratio for an isotropic 2D system can be easily expressed by the above elastic moduli, see e.g. [12].

$$\nu = \frac{B - \mu}{B + \mu}. \quad (7)$$

2.2. The simulation method

In the static case, which corresponds to the zero temperature, computation of elastic constants of (mechanically) stable structures can be done by searching for (local) energy minima of studied models. Simulations were carried out by searching for a minimum energy configuration of a system of N (usually of order of a few hundred) particles enclosed in periodic boundary conditions at a given volume, V . After the (local) equilibrium configuration of the particles was found, a very small external strain was applied to the system and a (new) configuration of minimal energy at the applied deformation was searched for. Then numerical differentiation of the energy with respect to the strain was carried out. Many runs (from ten to one thousand) with various initial conditions were performed for each set of parameters describing the studied systems to minimize the 'experimental' error. The details of the computations can be found in Ref. [10].

3. THE POISSON'S RATIOS OF THE STUDIED SYSTEMS

Below we describe three elastically isotropic systems which exhibit a certain, well controlled amount of disorder leading to *aperiodicity* of the structures. The first system [8] is a polydisperse model of monoatomic particles. The second system [9] consists of bi-atomic particles (dimers) arranged in a degenerate crystalline structure, similar to that described in Ref. [13]. The third system [10] is the system of tri-atomic particles (trimers) whose atoms exhibit non-zero polydispersity. In each of the studied cases only the nearest-neighbouring atoms of different particles interact through an inverse-power-potential.

We should stress here that in each of the cases considered a different kind of disorder is studied. This allows one for comparison of influence of various microscopic mechanisms on the Poisson's ratio. In the first model and in the third one, polydispersity is a measure of the disorder with respect to *periodic* (at zero polydispersity) atomic and molecular crystalline structures, respectively. It is worth to add that in the third model the studied system is aperiodic whereas the first model exhibits positive Poisson's ratio. In the second model, in which the reference molecular structure is an *aperiodic* solid of 'common' properties, disorder (of atomic posi-

tions) is introduced by changing the volume of the system.

3.1. 2D system of soft polydisperse discs

The system studied, shown in Fig. 1 and further referred to as the *polydisperse soft disc system*, consists of soft particles that interact only with their nearest neighbours through the interaction potential of the form

$$u(r_{ij}) = \varepsilon \left(\frac{d_i + d_j}{2r_{ij}} \right)^n, \quad (8)$$

where d_i and d_j are the diameters of the interacting particles and r_{ij} is the distance between their centres. The values of the diameters were generated [14] according to the Gauss distribution function

$$\rho(\sigma) = \frac{1}{\delta\sqrt{2\pi}} \exp\left[-\frac{(\sigma - \langle\sigma\rangle)^2}{2\delta^2} \right] \quad (9)$$

with the fixed size polydispersity parameter, δ , defined as:

$$\delta = \frac{(\langle\sigma^2\rangle - \langle\sigma\rangle^2)^{1/2}}{\langle\sigma\rangle}. \quad (10)$$

In the case when $\delta = 0$ the equation of state and the elastic constants of (mono-disperse) soft discs can be easily derived analytically:

$$\rho_0^{(m)} = n\varepsilon\sqrt{3a}^{-n-2}, \quad (11)$$

$$B_0^{(m)} = \left(\frac{n}{2} + 1 \right) \rho_0^{(m)}, \quad (12)$$

$$\mu_0^{(m)} = \left(\frac{n}{4} - \frac{1}{2} \right) \rho_0^{(m)}, \quad (13)$$

$$v_0^{(m)} = \frac{n+6}{3n+2}, \quad (14)$$

where n is the power of the potential and a is the distance between the centres of the particles. The system with $\delta = 0$ can be then thought of as a reference system for those of $\delta \neq 0$.

It can be seen in Fig.1 that the soft discs form nearly hexagonal lattice for which the elastic properties are isotropic for small deformations [1]. It is worth to stress that when the exponent n tends to infinity, the above system tends to the static (i.e.

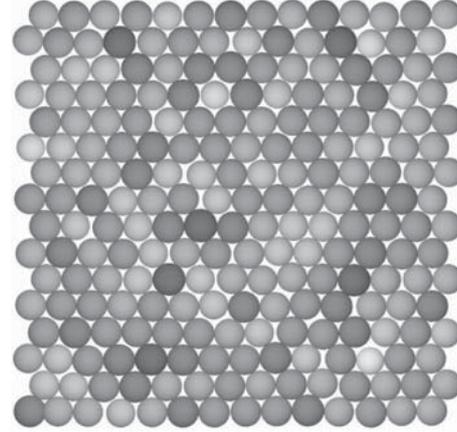


Fig. 1. Typical configuration of the studied system for $N = 224$ particles. Discs of different sizes are represented by different intensities of greyness.

zero temperature), polydisperse, hard disc system, studied in [15] at positive temperatures.

In Fig. 2 we show the dependence of the Poisson's ratio of polydisperse discs on the inverse of the exponent n for a few polydispersities. It can be seen that the Poisson's ratio grows with increasing polydispersity. It is also easy to notice that when $\delta \neq 0$ then the Poisson's ratio tends to its maximum value, +1, for $n \rightarrow \infty$.

3.2. 2D degenerate crystalline phase of soft dimers

In the system of soft dimers [9] each particle consists of two identical atoms between which there is a fixed distance σ . Each atom interacts with nearest-neighbouring atoms belonging to other particles through the potential

$$u(r_{ij}) = \varepsilon \left(\frac{\sigma}{r_{ij}} \right)^n, \quad (15)$$

where r_{ij} is the distance between atoms i ; j , and $\sigma=1$. When $n \rightarrow \infty$, the dimers become hard.

It is obvious that at close packing of the hard dimers their atoms form a closely packed periodic triangular lattice. However, the structure of the dimers is *not* periodic – the positive degeneracy entropy leads to aperiodic structure of the solid phase of the dimers in the whole density range where the solid phase is stable [16]. The thermodynamic properties of the aperiodic structure of hard dimers, further referred to as the degenerate crystal

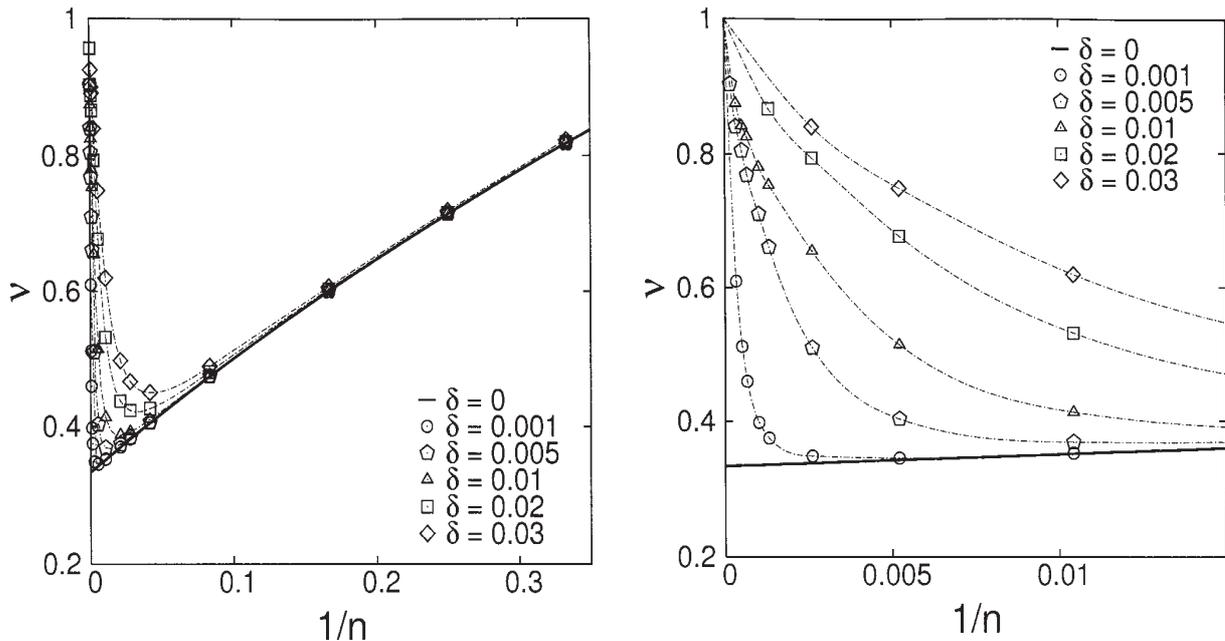


Fig. 2. The Poisson's ratio against the inverse of the exponent n for two-dimensional soft discs with different values of the polydispersity parameter δ : (a) in the range $n \in (3, \infty)$, (b) for $n \geq 96$. For all the studied systems $v_m^* = v/v^{(m)}_0 = 1$, where $v^{(m)}_0 = \sqrt{3}/2$. The thick continuous line shows the exact result for $\delta = 0$, see Eq. (14). The dotted lines are presented to guide the eye.

(DC), were discussed in detail in Ref. [17], their elastic properties at positive temperatures were studied only recently [18]. Typical configuration of the dimers in the DC phase at close packing is shown in Fig. 3.

The entropic argument leading to the DC phase is valid also in the case of nearest-neighbour soft interactions, i.e. when the atoms form triangular lattice. This corresponds to the volume of the system equal to $v_0 \equiv V/N = \sqrt{3}$. In the following we will compare the Poisson's ratio of the DC structure in which all the atoms form perfect triangular lattice to the Poisson's ratios of the DC structures whose volumes per particle slightly differ from v_0 . We should add that when $v \neq v_0$ then the atoms constituting dimers *cannot* form a perfect triangular lattice and are 'scattered' around the corresponding triangular lattice sites obtained by scaling the perfect lattice. Thus, the volume per the dimer in the latter structures can be used to measure disorder.

The Poisson's ratio for the system of the soft dimers is shown in Fig. 4 for some v^* . It can be seen there that the Poisson's ratio of the dimers at $v^* = 1$ is *lower* than that of the soft discs. It can be also seen that for $v^* \neq 1$ the Poisson's ratio for expanded or contracted systems much exceeds the values obtained for $v^* = 1$ when n is large enough. It

is worth to stress, however, that for uniformly expanded systems of soft dimers in certain range of n the Poisson's ratio can be (slightly) *smaller* than its value at v^* for the same n -s.

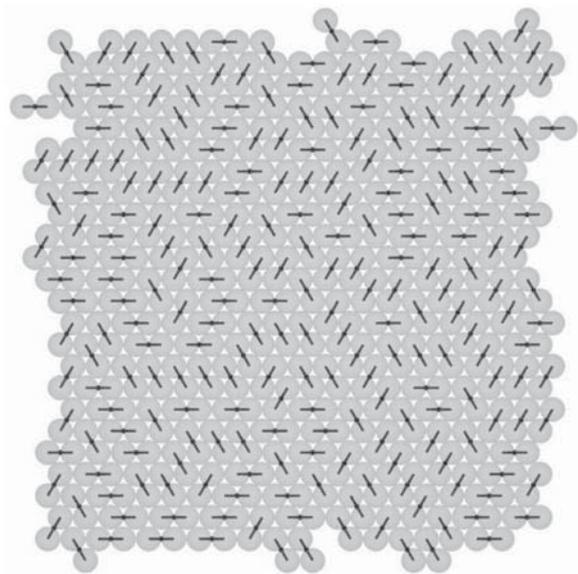


Fig. 3. Example of a structure representing the DC phase for $N = 240$ molecules at $v^* \equiv v/v_0 = 1$.

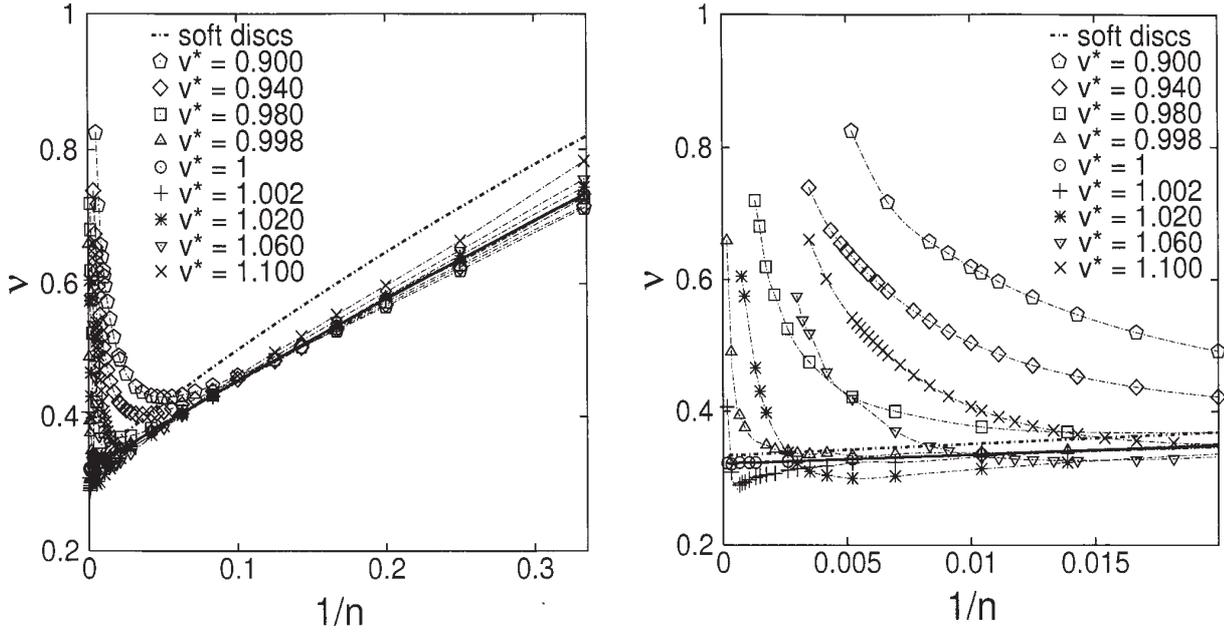


Fig. 4. Poisson's ratio of the DC structure of soft dimers as the function of the inverse of the exponent n : (a) in the range $n \in (3, \infty)$, (b) for $n \geq 50$. Continuous line shows the Poisson's ratio for the system at $v^* = 1$, where $v^* = V/V_0$. Thick dashed line shows results for the triangular lattice of identical soft discs ($\delta = 0$) at $v^* = 1$.

3.3. 2D system of soft polydisperse trimers

In the system of soft trimers [10] each trimer is build of three atoms forming a rigid equilateral triangle of unit side. In contrast to the dimers, considered in the previous paragraph, the atoms forming trimers are not identical. Their diameters were generated according to the same Gaussian distribution as in the case of polydisperse discs, see Eqs. (9) and (10). The nearest-neighbouring atoms of different molecules interact by the same potential as the polydisperse disc, see Eq. (8).

As in the case of the mono-disperse discs, the system consisting of perfect trimers is periodic and can be solved analytically [12]

$$\rho_0^{(t)} = \frac{6n\sqrt{4r^2 - 1}}{r^2(3 + \sqrt{12r^2 - 3})}, \quad (16)$$

$$B_0^{(t)} = \frac{3n \left((2+n)(4r^2 - 1)^{\frac{3}{2}} + \sqrt{3}(4(1+n)r^2 - 2 - n) \right)}{4r^4(3 + \sqrt{12r^2 - 3})}, \quad (17)$$

$$\mu_0^{(t)} = \frac{3n(\sqrt{3n} + (n-2)\sqrt{4r^2 - 1})}{2r^2(3 + \sqrt{12r^2 - 3})}, \quad (18)$$

$$v_0^{(t)} = \frac{3(2r^2 - 1)(2+n) + \sqrt{12r^2 - 3}(2r^2(6+n) - 2 - n)}{(3 + \sqrt{12r^2 - 3})(r^2(4 + 6n) - 2 - n)}, \quad (19)$$

where r is the radius of the atoms.

An example of a typical structure of the trimers of high anisotropy is shown in Fig. 5. In contrast to the two models discussed previously, the perfect trimers of this anisotropy exhibit negative Poisson's ratio for the studied range of exponents n [12].

In Fig. 6 the Poisson's ratio of the trimers presented in the previous figure is shown as a function of n^{-1} . As one can see, the qualitative behaviour of the Poisson's ratio is very similar to that observed in the case of the polydisperse discs.

4. SUMMARY AND CONCLUSIONS

The investigations discussed in this work revealed essential influence of disorder on the Poisson's ra-

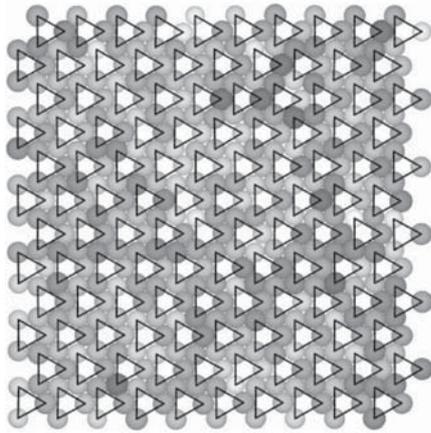


Fig. 5. Example of a studied structure of polydisperse trimers. Disks of different sizes are represented by different intensities of greyness.

tio in 2D elastically isotropic systems. A few kinds of static disorder, leading to aperiodicity of the system ground states were studied: (a) polydispersity of isotropic particles, (b) polydispersity of anisotropic particles (triatomic molecules), and (c) misfit between the lattice constant (which can be varied) and the fixed intramolecular bonds, i.e. the distances between centres of 'atoms' forming the dimers. In each of the studied cases an increase of the

Poisson's ratio was observed with increasing hardness of the potential for short-range interactions. It was also observed that the Poisson's ratio grows with increasing disorder for short-range, steeply varying potentials.

Increase of the Poisson's ratio with increasing disorder has been observed in systems with vacancies both in two [19] and in three dimensions both for atomic systems [20] and for molecular ones [21, 22]. Thus, it is attractive to conjecture that such a behaviour is a typical one, at least for short-range interactions. Studies of other model crystals with defects constitute a simple way to recognize the range of thermodynamic and structural parameters for which this conjecture is valid.

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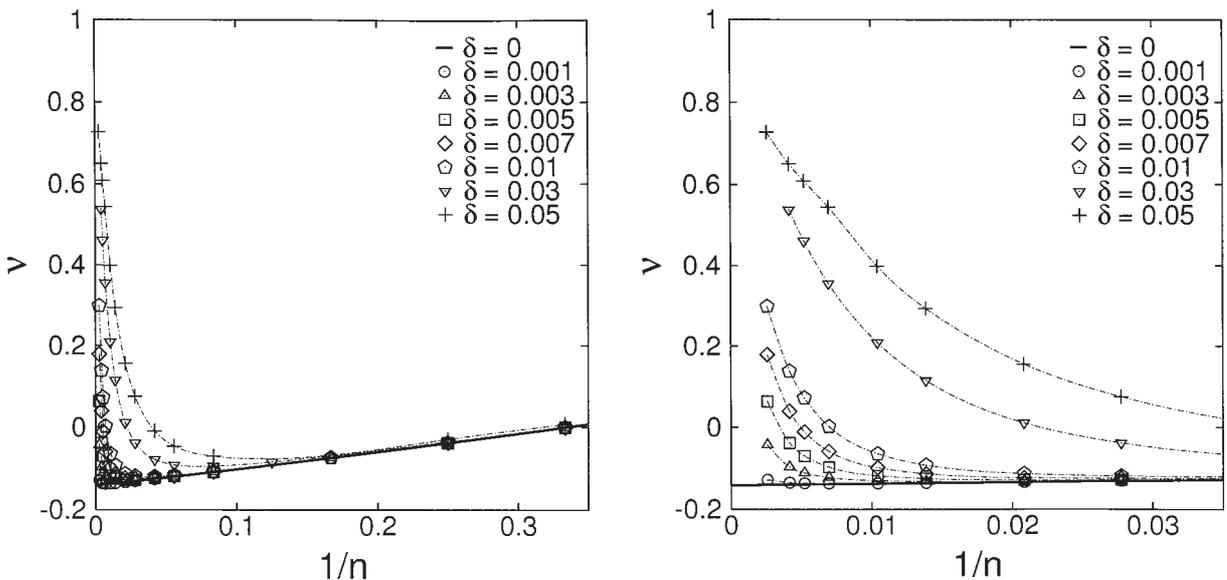


Fig. 6. The Poisson's ratio ν with respect to the exponent n of the potential for the soft polydisperse trimer system: (a) in the range $n \in (3, \infty)$, (b) for $n \geq 36$. The thick continuous line presents the theoretical results obtained from Eq. (19). For all the studied systems $\nu_t^* \equiv \nu / \nu^{(t)_0} = 1$, where $\nu^{(t)_0}$ corresponds to the close packing of perfect trimers of the studied anisotropy.

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