Phase diagram of the system with the repulsive shoulder potential in two dimensions: Density functional approach

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H I G H L I G H T S

- Melting scenarios of two dimensional repulsive shoulder potential systems are studied.
- The phase diagram is calculated using the density functional theory of freezing.
- We show that at low densities the system melts though continuous transition.
- At high densities melting occurs through the first order transition.

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In the framework of the density functional theory of freezing proposed in our previous works, we calculate the phase diagram of two-dimensional system of particles interacting through the repulsive shoulder potential. This potential consists of the hard core and repulsive shoulder of the larger radius. It is shown that at low densities the system melts through the continuous transition in accordance with the Kosterlitz–Thouless–Halperin–Nelson–Young (KTHNY) scenario, while at high densities the conventional first order transition takes place.

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A large number of papers studying the melting transition in two dimensions have been published during last decades. They include results of real experiments, computer simulations and various theoretical approaches. This is dictated by the growing interest to the behavior of the nanoconfined systems. Confining drastically changes the spatial distribution and the ways of dynamic rearrangement of the molecules in the system. The confined fluids microscopically relax and flow with characteristic times that differ from the bulk fluids. These effects play important role in the thermodynamic behavior of the confined systems and can considerably change the topology of the phase diagram. In general, the motivation for the study of the confined systems follows from the fact that there are a lot of real physical, chemical and biological processes which drastically depend on the properties of such systems [1–6].

It is not surprising that the spatial ordering of molecules depends on the dimensionality of the space to which it is confined. Mermin [7] has shown that in two dimensions (2D) the long-range crystalline order cannot exist because of the

thermal fluctuations and transforms to the quasi-long-range order. On the other hand, the real long range bond orientational order does exist in this case. At high temperatures one can find the conventional isotropic fluid.

The melting scenario in two dimensions is a subject of long lasting controversy. Now it is widely believed that the Kosterlitz, Thouless, Halperin, Nelson, and Young theory (KTHNY theory) [8–11] correctly describes the melting transition in 2D. In the framework of the KTHNY theory the two-dimensional melting occurs in the way which is fundamentally different from the melting transition of three-dimensional systems. In 2D, the bound dislocation pairs dissociate at some temperature T_m transforming the quasi-long range translational order into the short-range one, and the long-range orientational order into the quasi-long range one. The new phase with the quasi-long range orientational order is called the hexatic phase. After consequent dissociation of the disclination pairs at some temperature T_i the system transforms into the isotropic liquid. Both transitions are continuous, in contrast with the conventional first order three dimensional melting.

The unambiguous confirmations of the KTHNY theory have been obtained, for example, from the recent experiments on the colloidal model system with repulsive magnetic dipole–dipole interaction [12–16]. On the other hand, the first-order melting in 2D is also possible [17–24]. In Refs. [23,24] it was shown that at low disclination core energy system can melt through one first-order transition as a result of the dissociation of the disclination quadrupoles.

KTHNY theory is independent on the pair potential of the system and seems universal, however, numerous experimental and simulation studies demonstrate the controversial results: the systems with very short range or hard core potentials melt through weak first-order transition, while the melting scenarios for the soft repulsive particles favor the KTHNY theory [2,25–50].

In Refs. [21,22] the phenomenological theory was proposed which explains on the qualitative level the possible interplay between the first-order and continuous melting transitions in 2D. Here we repeat some ideas from these works because they will be used in what follows. As it was mentioned above, in 2D the long range translational order cannot exist due to the thermal fluctuations. It is well known that in the 3D case the melting transition order parameters are given by the Fourier components $\rho_{\mathbf{G}}$ of the expansion of the one-particle distribution function in a Fourier series in reciprocal lattice vectors $\mathbf{G}$ (see, for example, reviews [51,52]).

In 2D, because of the thermal fluctuations, the order parameters $\rho_{\mathbf{G}}$ are no more the constants over the system and slowly vary at distances of the order of G^{-1}. In this case the order parameter can be written in the form $\rho_{\mathbf{G}}(\mathbf{r})$ and has the amplitude and the phase. Taking into account that in 2D the phase fluctuates most strongly, one can neglect the fluctuations of the amplitude and write the order parameter in the form:

$$\rho_{\mathbf{G}}(\mathbf{r}) = \rho_{\mathbf{G}} e^{i\mathbf{G}u(\mathbf{r})}. \tag{1}$$

Here $u(\mathbf{r})$ has the meaning of the displacement field, which, in general, can be decomposed into the smooth part corresponding to the phonon field, and singular part, which can be interpreted as the Kosterlitz–Thouless vortices [8] or dislocations.

Taking into account the long range fluctuations, one can write the phenomenological Ginzburg–Landau–Wilson expansion in the most general form:

$$\Delta F = \frac{1}{2} \int d^2 r \sum_{\mathbf{G}} \left[A|\mathbf{G} \times \nabla \rho_{\mathbf{G}}|^2 + B|\mathbf{G} \cdot \nabla \rho_{\mathbf{G}}|^2 + C|\rho_{\mathbf{G}}(\mathbf{G} \cdot \nabla)\rho_{\mathbf{G}}| \right]$$
$$+ \frac{1}{2} a_T \sum_{\mathbf{G}} |\rho_{\mathbf{G}}|^2 + b_T \sum_{\mathbf{G}_1 + \mathbf{G}_2 + \mathbf{G}_3 = 0} \rho_{\mathbf{G}_1} \rho_{\mathbf{G}_2} \rho_{\mathbf{G}_3} + O(\rho^4). \tag{2}$$

ΔF is the difference of the free energies of crystal phase and isotropic liquid. The terms in the integrand in the expansion (2) correspond to all possible isotropic combinations which contain the gradients of the order parameter. This expansion was proposed in Ref. [53] in order to obtain the microscopic expressions for the Lame coefficients in the elastic energy. After substitution of Eq. (1) into (2), it may be shown that the first term in the expansion (2) is expressed in terms of the derivatives of $\partial u_i / \partial x_i$ and has the form of the free energy of a deformed solid [19,20,53] and can be used in the framework of the KTHNY theory [9–11] with the obtained microscopic expressions for the Lame coefficients. It should be noted, that the Lame coefficients are proportional to the squared modulus of the order parameter (1).

As it was discussed in detail in Refs. [21,22], with the help of Eq. (2), the 2D melting scenario can be described in the following way. The modulus of the order parameter becomes zero through the first-order phase transition at the mean-field temperature T_{MF}. On the other hand, if the order parameter modulus is nonzero, at temperature T_m the singular fluctuations of the phase of the order parameter (vortices), which corresponds to the free dislocations, appear in accordance with the standard Kosterlitz–Thouless paradigm, and the system melts through the continuous transition. So, there are two possibilities: (i) $T_m < T_{MF}$, and the system melts through the continuous Kosterlitz–Thouless transition; (ii) $T_m > T_{MF}$, the system melts through the first-order transition.

In our previous publications the density functional approach for the description of the 2D melting was proposed [19,20] and it was shown that the hard disk system melts through the first order phase transition, while in the 2D Coulomb system the melting transition occurs in accordance with the KTHNY scenario. In Refs. [21,22] the density functional calculations were used for the description of the melting transition in the 2D square-well system. It was shown that this system can demonstrate both first-order and continuous melting transitions depending on the width of the attractive well.

In the present paper we extend our previous results to the melting transition in the 2D square-shoulder system in order to study the influence of the width of the shoulder on the phase diagram. The potential is given by the equation:

$$U(r) = \begin{cases} \infty, & r \leq d \\ \varepsilon, & d < r \leq \sigma \\ 0, & r > \sigma, \end{cases} \tag{3}$$

where d is the diameter of the hard core, σ is the width of the repulsive step, and ε its height. As it was discussed before [54,55], in the low-temperature limit $\tilde{T} \equiv k_B T/\varepsilon \ll 1$ the system reduces to a hard-disk system with hard-disk diameter σ. At the same time, in the limit $\tilde{T} \gg 1$ the system reduces to a hard-disk model with a smaller hard-disk diameter d. In this case, melting at high and low temperatures are described by the simple hard-disk melting curve $P = cT/\sigma'^2$, where σ' is the hard-disk diameters (σ and d, respectively). A crossover from the low-T to high-T melting behavior takes place for $\tilde{T} = \mathcal{O}(1)$. The precise form of the phase diagram depends on the ratio $s \equiv \sigma/d$. For large enough values of s one should expect to obtain the melting curve with a maximum that should disappear as $s \to 1$ [54,55]. In what follows we will use the reduced units $r' = r/d$, $\rho' = \rho/d^2$ and omit tilde.

The different smoothed versions of the potential (3) (core softened potentials) were discussed recently in order to study the water-like anomalies which appear due to the existence of two length scales in the potential [55–62].

The melting scenarios of the systems with the smoothed versions of the potential (3) in two dimensions were studied in Refs. [31–33] in the framework of computer simulations. It was shown, that at small width of the soft core, when the system behaves like an ordinary soft disk system, melting occurs through one weak first order transition. However, with increasing the width of the repulsive shoulder, the phase diagram becomes much more complex. As in Ref. [25], we found that the phase diagram consists of three different crystal phases, one of them with square symmetry and the other two triangular. At low densities, when the soft core of the potential is effective, melting of the triangular phase is a continuous two-stage transition, with an intermediate hexatic phase, in accordance with the KTHNY scenario for this melting transition. At high density part of the phase diagram one finds the square and triangular phases, which melt through one first-order transition. The thermodynamic and dynamic anomalies do exist in this case, however, the order of these anomalies is inverted in comparison with the three-dimensional case [33].

At the same time, in Ref. [4] the phase diagram of a square-shoulder square-well potential was studied in two dimensions. It has been previously shown that this potential exhibits liquid anomalies consistent with a metastable liquid-liquid critical point [63]. It was shown that the melting occurs through the first order transition, despite a small range of metastability.

The first order transition temperature T_{MF} can be estimated from the Helmholtz free energy F of the solid calculated in the framework of the density functional theory of freezing [19–22,53]. Because our main purpose is to obtain a qualitative description of the melting transition in the system with the repulsive step potential, we use the simplest but correct enough version of the density functional theory of freezing (DFTF), based on the local density functional [19–22,51,52]. In this case the local density of the solid, $\rho(\mathbf{r})$, can be represented as localized Gaussians (of width $1/\alpha^{1/2}$) at lattice sites. The order parameters, which are the Fourier transforms of the local density of the solid, have the form $\rho_{\mathbf{G}} = \rho \exp(-G^2/4\alpha)$, where $\rho = \int d\mathbf{r}\rho(\mathbf{r})/V$ is the average density. The difference of the Helmholtz free energies of the solid and liquid phases ΔF is given by:

$$\beta \Delta F = \int d\mathbf{r}\rho(\mathbf{r}) \ln[\rho(\mathbf{r})/\rho] - \frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}' \, c^{(2)}(|\mathbf{r} - \mathbf{r}'|, \rho)[\rho(\mathbf{r}) - \rho][\rho(\mathbf{r}') - \rho], \tag{4}$$

where $c^{(2)}(|\mathbf{r} - \mathbf{r}'|, \rho)$ is the direct correlation function [64], $\beta = 1/k_B T$. The localization parameter α is fixed by minimizing the total free energy with respect to it. This version of DFTF presents a qualitatively correct description of the hard sphere melting transition in 3D [65]. The more involved versions of the density functional theory of freezing were proposed later (see, for example, reviews [51,52]). It should be mentioned the weighted-density approximation (WDA) [66,67] and effective liquid approximation (ELA) [51,68]. Both these approximations improve the results for the melting parameters of the 3D hard spheres [51,52] and can be applied in the two-dimensional case. For example, in our previous works [19–22] ELA was successfully used for the calculations of the melting parameters of the systems with the hard disks, Coulomb, Yukawa and square-well potentials. However, the application of ELA to the system with the repulsive shoulder potential (3) is difficult because in this case the first peak of the static structure factor is split. In the present paper we consider the simplest form of the DFTF as the first approximation which, however, gives rather correct results for the melting parameters of the hard disks (see below).

In principle, the parameters of the first order melting transition should be determined from Eq. (4) using the double tangent construction, however, for the approximate qualitative description of the phase diagram it seems sufficient to apply the equation $\Delta F = 0$ in order to determine T_{MF}.

The temperature T_m can be determined from the KTHNY criterion [9–11] which determines the instability of the crystal lattice with respect to the appearance of free dislocations:

$$K(T_m) = \frac{a_0^2}{k_B T_m} \frac{4\mu(T_m)(\mu(T_m) + \lambda(T_m))}{2\mu(T_m) + \lambda(T_m)} = 16\pi, \tag{5}$$

where $\mu(T)$ and $\lambda(T)$ are the Lame coefficients and a_0 is the lattice constant for the triangular lattice: $a_0^2 = 2/(\sqrt{3}\rho)$.
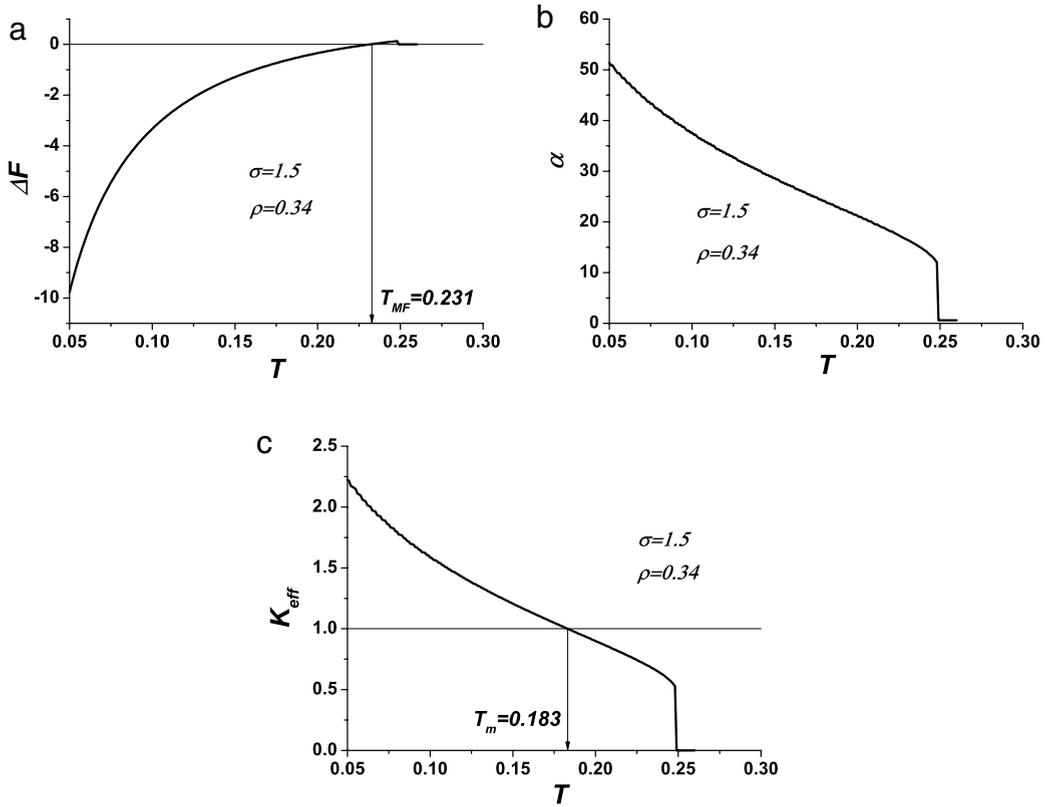
Fig. 1. ΔF (a), α (b), and $K_{eff} = K/16\pi$ (c) as functions of temperature for $\rho = 0.34$.

Expressions for the Lame coefficients have the form [21,22]:

$$\mu = \frac{k_B T}{16\rho} \sum_G \rho_G^2 m_G G^2 (\gamma_G + 2\delta_G), \tag{6}$$

$$\lambda = \frac{k_B T}{16\rho} \sum_G \rho_G^2 m_G G^2 (\gamma_G - 6\delta_G) + k_B T \rho (1 - \rho \tilde{c}^{(2)}(0)), \tag{7}$$

where

$$\gamma_G = 2\pi\rho \int r^3 \, dr \, c^{(2)}(r; \hat{\rho}) J_0(Gr),$$

$$\delta_G = 2\pi\rho \int r^3 \, dr \, c^{(2)}(r; \hat{\rho}) J_1(Gr)/(Gr),$$

and $J_0(x)$ and $J_1(x)$ are the Bessel functions, m_G is the number of reciprocal lattice vectors with the same length, and $\tilde{c}^{(2)}(q)$ is the Fourier transform of the direct correlation function. Expressions (6) and (7) were obtained in Ref. [53] (see also Refs. [19–22]) using the coincidence of the long range asymptotic behavior of the density correlation function obtained with the help of the Hamiltonian (2) and calculated from the exact nonlinear equations for the many particle correlation functions [69,70].

For the further calculations one needs an approximate expression for the direct correlation function. We use the simple approximation for the direct correlation function [64] of the hard-core system, suggested by Lovett [71] (see also Refs. [21,22,72,73]):

$$c^{(2)}(r, \rho) = \begin{cases} c_{HD}^{(2)}(r, \rho), & r \leq d \\ -\dfrac{\phi(r)}{k_B T}, & r > d, \end{cases} \tag{8}$$

where $c_{HD}^{(2)}(r, \rho)$ is the hard disks direct correlation function and $\phi(r)$ is the repulsive shoulder or attractive part of the potential. This approximation should be a good one when $-\frac{\phi(r)}{k_B T}$ is small. The approximation, though rough, is similar in
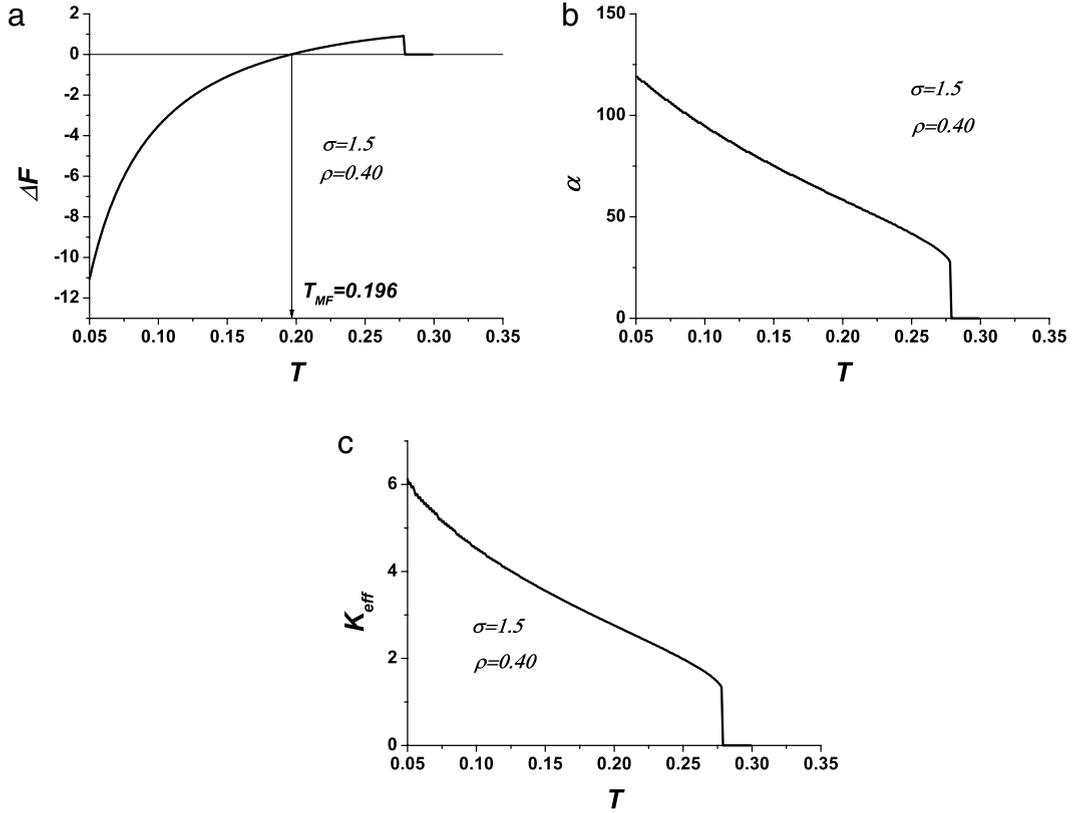
Fig. 2. ΔF (a), α (b), and $K_{eff} = K/16\pi$ (c) as functions of temperature for $\rho = 0.40$.

spirit to the mean spherical model approximation which has been found to be a good approximation in many cases [64]. In the case of the potential (3), Eq. (8) takes the form:

$$c^{(2)}(r, \rho) \approx \begin{cases} c_{HD}^{(2)}(r, \rho), & r \leq d \\ \dfrac{-\varepsilon}{k_B T}, & d < r \leq h \\ 0, & r > h. \end{cases} \tag{9}$$

For $c_{HD}^{(2)}(r, \rho)$ we use the approximate analytic equation obtained in Refs. [74,75]:

$$c_{HD}^{(2)}(x; \eta) = -\left[\frac{\partial}{\partial \eta} (\eta Z(\eta)) \right] \Theta(1-x) \times \left\{ 1 - a^2 \eta + \frac{2}{\pi} a^2 \eta \left[\arccos \frac{x}{a} - \frac{x}{a} \left(1 - \frac{x^2}{a^2} \right)^{1/2} \right] \right\},$$

$$Z(\eta) = (1 + c_2 \eta^2)/(1 - \eta)^2,$$

$$a = (2 + \eta \alpha_2(\eta))/(1 + \eta + \eta \alpha_2(\eta)), \tag{10}$$

where $c_2 = 0.128$; $\alpha_2(\eta) = -0.2836 + 0.2733\eta$; $\eta = \pi \rho d^2/4$.

In Figs. 1 and 2 we represent the behavior of ΔF (see Eq. (2)), localization parameter α, and $K_{eff} = K/16\pi$ (Eq. (5)) as a function of T for $\sigma = 1.5$ and $\rho = 0.34$ (Fig. 1) and $\rho = 0.4$ (Fig. 2). One can see, that for $\rho = 0.34$ the solution of equation $\Delta F = 0$ which determines the first-order transition temperature T_{MF}, is $T_{MF} = 0.231$ (Fig. 1(a)), while the solution of the equation $K_{eff} = 1$ (Fig. 1(c)) $T_m = 0.183 < T_{MF}$. As it was discussed above, in this case the melting should occur in accordance with the KTHNY scenario. From Fig. 1(b) one can conclude that the localization parameter α is well defined till the limit of metastability of the crystal lattice $T_{met} = 0.248$. On the other hand, for $\rho = 0.40$ the situation is different. In this case $T_{MF} = 0.196$ while the equation $K_{eff} = 1$ does not have solution till the limit of metastability $T_{met} = 0.278$. In this case melting occurs through the first order transition.

At high densities there is only weak dependence of the melting density on temperature (see below). In this case, in calculations it is more convenient to fix the temperature and change the density. The typical results are shown in Fig. 3 for $\sigma = 1.5$ and $T = 1.0$. One can see that at high densities for $T = 1.0$ there is the first order melting transition at $\rho_{MF} = 1.015$. The equation $K_{eff} = 1$ does not have solution till the limit of metastability $\rho_{met} = 1.009$.
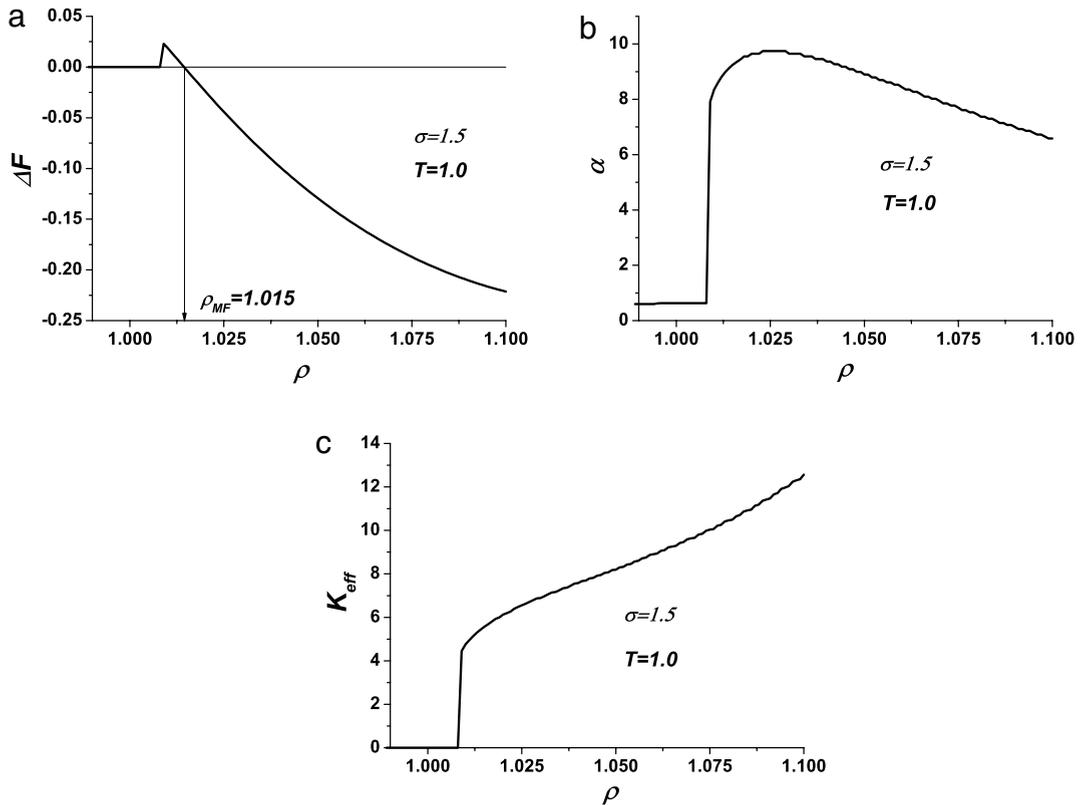
Fig. 3. ΔF (a), α (b), and $K_{eff} = K/16\pi$ (c) as functions of density for $T = 1.0$.
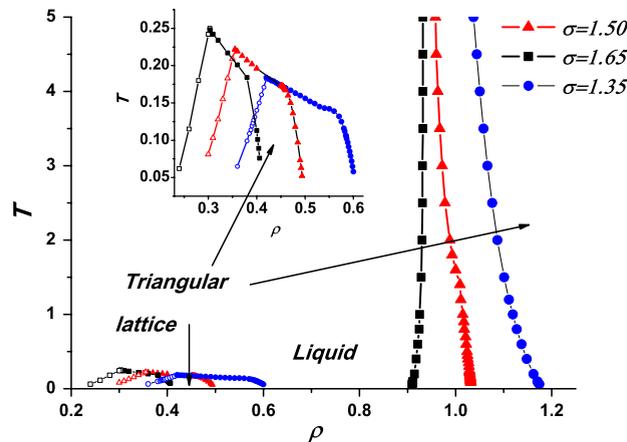

Fig. 4. Phase diagram of the system with the potential (3) for three repulsive shoulder widths: $\sigma = 1.50$ (triangles), $\sigma = 1.35$ (circles), $\sigma = 1.65$ (squares). Open symbols correspond to the continuous transitions, while the bold symbols mark the first order transitions. The solid phase corresponds to the triangular lattice.

In Fig. 4 we present the resulting phase diagram for three widths of the repulsive shoulder in the potential (3): $\sigma = 1.50$, $\sigma = 1.35$, and $\sigma = 1.65$. In accordance with the qualitative discussion after Eq. (3), the phase diagram consists in two parts − the low density triangle lattice with the maximum on the melting curve and the high density triangle lattice. It is interesting that at lowest density part of the phase diagram the KTHNY scenario takes place, while with the increasing density the melting becomes the first order transition. Taking into account the fact, that with increasing the density the hard core of the potential (3) becomes effective, one can conclude that this result is consistent with the mentioned above possibility that the systems with soft potentials probably melt in accordance with the KTHNY scenario, while the hard core systems melt through the first order transition. It should be noted that with increasing temperature the system has to behave more and more closely to the hard disk system. There are different estimates for the melting density of hard disk systems

[19,20,35,36,38] which vary from $\rho = 0.905$ to $\rho = 0.933$. One can see that despite very simple approximations (4), the results presented in Fig. 4 for high temperatures, are in good agreement with previous estimates. For example, the melting density at $T = 1000$ is $\rho = 0.9326$. It should also be noted, that for the potential (3) the approximation given by Eq. (4) works well in the limit of high densities which corresponds to the hard disk system.

We also considered the possible square lattice but found that it is less stable than the triangle lattice for all densities.

It should be noted that the similar behavior was found in computer simulation of the smoothed version of the potential (3) [31–33]. As it was mentioned in the introduction, in Refs. [31–33] it was shown that at low densities melting occurs through two continuous transitions with the intermediate hexatic phase, however, at high densities only first order transition takes place. As in the present case, the "gap" between the two parts of the phase diagram takes place which increases with increasing the width of the repulsive shoulder. In principle, some crystal lattice can exists in this range of densities at low enough temperatures, however, we could not find it in the present work. Another open question exists for further study. It is related with the crossover from the continuous to first order transition in the phase diagram in Fig. 4. It must be the tricritical point on the melting line, however, in the present study we could give only rough enough estimate for the location of this point without investigation of the properties of this point.

In conclusion, in the present study we consider the melting transition of the repulsive shoulder potential system (3). In the framework of the density functional theory of freezing we calculate the phase diagram and show that it consists of two parts with different melting scenarios (see Fig. 4). At low densities the system melts through the continuous transition in accordance with the Kosterlitz–Thouless–Halperin–Nelson–Young (KTHNY) scenario, while at high densities the conventional first order transition takes place. Taking into account the fact, that with increasing the density the hard core of the potential (3) becomes effective, one can conclude that this result is consistent with the possibility that the systems with soft potentials probably melt in accordance with the KTHNY scenario, while the hard core systems melt through the first order transition.

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