The role of attraction in the phase diagrams and melting scenarios of generalized 2D Lennard-Jones systems

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Monolayer and two-dimensional (2D) systems exhibit rich phase behavior, compared with 3D systems, in particular, due to the hexatic phase playing a central role in melting scenarios. The attraction range is known to affect critical gas-liquid behavior (liquid-liquid in protein and colloidal systems), but the effect of attraction on melting in 2D systems remains unstudied systematically. Here, we reveal how the attraction range affects the phase diagrams and melting scenarios in a 2D system. Using molecular dynamics simulations we considered the generalized Lennard-Jones system with a fixed repulsion branch and different power indices of attraction, from long-range dipolar to short-range sticky-spheres-like. A drop in the attraction range has been found to reduce the temperature of the gas-liquid critical point, bringing it closer to the gas-liquid-solid triple point. At high-temperatures, attraction does not affect the melting scenario that proceeds through the cascade of solid-hexatic (Berezinski-Kosterlitz-Thouless) and hexatic-liquid (first-order) phase transitions. In the case of dipolar attraction, we observed two triple points, inherent in a 2D system: hexatic-liquid-gas and crystal-hexatic-gas, the temperature of the crystal-hexatic-gas triple point is below the hexatic-liquid-gas triple point. This observation may have far-reaching consequences for future studies, since phase diagrams determine possible routes of self-assembly in molecular, protein, and colloidal systems, whereas the attraction range can be adjusted with complex solvents and external electric or magnetic fields. The results obtained may be widely used in condensed matter, chemical physics, materials science, and soft matter.

I. INTRODUCTION

Understanding phase transitions in 2D systems has prominent importance in a number of areas, from photonics and electronics, to novel materials and biotechnologies, since the knowledge on phase behavior opens a way to design systems with desired properties. Despite many studies, the fundamental questions here are still related to the effect of particular interaction between individual particles on their collective behavior. For classical systems, one of the simplest models capable of reproducing their behavior, including gas, liquid, and solid phases, is the Lennard-Jones (LJ) system. The LJ model is widely used for analysis of behavior in molecular, protein, polymer, emulsion, and colloidal soft matter. The generalized LJ potential (or the Lennard-Jones potential, where indices \( n \) and \( m \) are responsible for the algebraic branches of repulsion and attraction, see below) is a suitable model for studies, aimed to reveal the effects of repulsion and attraction on liquids and solids, and the phase transitions between them.

Today, it has been established that 2D melting scenarios depend on repulsion softness, providing the following microscopic scenarios of 2D melting:

1. the Berezinskii-Kosterlitz-Thouless-Halperin-Nelson-Young (BKTHNY) theory, according to which melting occurs via two continuous transitions with an intermediary hexatic phase with quasi-long-range orientational order and short-range translational order; (ii) melting through a first order phase transition; (iii) two-step melting, including a continuous (Berezinski-Kosterlitz-Thouless, BKT) crystal-hexatic phase transition and a first-order phase transition between the hexatic phase and isotropic liquid. The second and third scenarios are inherent in hard-sphere-like systems, whereas the first one was observed for soft repulsion between particles. It has been established unambiguously that the softness of repulsion affects melting scenarios, thermodynamics and excitation spectra in monolayer systems. However, to the best of our knowledge, the role of attraction in the melting scenario of monolayer systems remains unstudied systematically.

LJ interactions were among the first systems studied to understand the role of attraction in melting. However, a lot of reported results on the critical point and melting scenario for 2D LJ crystals still remain questionable. For instance, to provide critical temperature depending on the truncation radius, numerical simulations of a vapor-liquid curve performed in the Gibbs ensemble were reported in Ref. For critical temperature and density, the authors obtained \( T_c = 0.515 \pm 0.002 \) and

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was observed for all temperatures considered in Ref.\textsuperscript{14}, whereas the authors expected to observe the BKTHNY scenario at higher temperatures. However, at some parameters of potential softness, two continuous transitions were observed already at low temperatures in the presence of long-range attraction.

The role of attraction can be tested experimentally in colloidal systems, known for a long time as model systems demonstrating a wide range of “molecular-like” phenomena, in particular, crystallization and melting\textsuperscript{31,39} solid-solid phase transitions\textsuperscript{30,62} condensation and critical phenomena\textsuperscript{63,65} caused by relatively short-range attractive depletion forces\textsuperscript{66}. These collective phenomena can be visualized in real-time with spatial resolution of individual particles. Long-range dipolar attraction \( \propto 1/r^3 \) in colloidal systems can be induced and controlled \textit{in situ} with in-plane rotating magnetic, \textit{opt}ic, or electric fields. Using conically-rotating magnetic or electric fields with magic angles, Van-der-Waals-like attraction can be created \( \propto 1/r^6 \) with “magic” fields\textsuperscript{63,65}. Recently, tunable interactions have been achieved by using spatial hodographs of an external electric or magnetic field\textsuperscript{68} by engineering the internal structure\textsuperscript{68} and geometry\textsuperscript{69} of colloidal particles.

In the present paper, we studied the role of the attraction range in the phase behavior and melting scenarios of a 2D system. Using MD simulations, we considered a generalized Lennard-Jones system with a fixed repulsion branch and different attraction, from long-range dipolar attraction to short-range sticky-spheres-like. A decrease in the attraction range is found to suppress the temperature of the gas-liquid (liquid-liquid in the case of colloid and protein systems) critical point. We found that attraction does not affect melting at high temperatures, occurring through the cascade of solid-hexatic (BKT) and hexatic-liquid (first-order) phase transitions. Surprisingly, at moderate temperatures we observed two triple points, hexatic-liquid-gas and crystal-hexatic-gas. The crystal-hexatic-gas triple point for the case of isotropic dipolar attraction has been discovered to be below the hexatic-liquid-gas triple point.

## II. SYSTEM AND METHODS

### A. MD details

We studied a system of particles interacting via the generalized Lennard-Jones potential (LJ\textsubscript{m-n}):

\[
U_{nm}(r) = \frac{\epsilon}{n-m} \left[ m \left( \frac{\sigma}{r} \right)^n - n \left( \frac{\sigma}{r} \right)^m \right],
\]

where \( n \) and \( m \) are the indices of repulsive and attractive branches, respectively, and \( \sigma \) and \( \epsilon \) are the characteristic length of interaction and the depth of the potential well. The potential \( U \) has minimum \(-\epsilon\) at \( r/\sigma = 1 \). In what follows, we normalized the distances and energies to \( \sigma \) and

\[
\rho_c = 0.355 \pm 0.003 \text{, respectively, for the full potential; and } T_c = 0.459 \pm 0.001 \text{ and } \rho_c = 0.35 \pm 0.01 \text{ for the truncated and shifted potential at } 2.5 \sigma. \text{ Contradictory melting scenarios of the triangular crystal were reported in the early work\textsuperscript{33,39}, including two continuous transitions with an intermediate hexatic phase according to the BKTHNY theory\textsuperscript{31} and a first-order transition\textsuperscript{35,39}. } 

Thanks to growth of computing capabilities, simulations of large systems (\( \gtrsim 10^5 \) particles) have recently provided new results on 2D melting of LJ crystals and related systems. Simulations of the systems followed by analysis of their equation of state and long-range asymptotics of the translational correlation function (that accurately provides the stability limit of the crystal) allowed identifying the melting scenarios unambiguously. For instance, a change in the melting scenario was reported in Ref.\textsuperscript{14} where the authors studied 2D systems of particles interacting via generalized LJ potential with different repulsive branches (\( \propto 1/r^{12} \) and \( \propto 1/r^{64} \)). The scenario was found to occur through first-order phase transitions at low temperatures and via two continuous BKT transitions (according to the BKTHNY theory) at high. An LJ system at high temperatures is typically assumed to be close to soft repulsive disks 1/r\textsuperscript{12}, but such extrapolation to a melting scenario contradicts the results of Ref.\textsuperscript{14} wherein the soft disks 1/r\textsuperscript{n} with \( n > 6 \) were shown to melt according to the third melting scenario. The Mayer-Wood loop, inherent in first-order transition, is assumed to disappear at high temperatures with an increase in the system size. However, the explanation of the effect by finite-size scaling seems unconvincing: With an increase in the system size, the loop should flatten and ultimately approach the plateau\textsuperscript{12,41}.

A first-order hexatic-liquid transition and a continuous crystal-hexatic BKT transition at high temperatures and one first-order crystal-liquid transition at low temperatures were identified in Ref.\textsuperscript{32} for 2D LJ particles. The results of numerical simulation of a 2D LJ system and attractive polygons (squares, pentagons and hexagons) of the same authors in Ref.\textsuperscript{14} revealed the role of attraction in a melting scenario. Thus, at low temperatures where the role of attraction is dominant all systems melt via first-order transition due to suppression of the hexatic phase. At high temperatures LJ disks melt in accordance with the third scenario, the same as soft disks\textsuperscript{14,15,19} whereas hexagons and squares do according to the BKTHNY theory with participation of the hexatic and tetratic phases, respectively. The melting scenario of pentagons does not change with an increase in temperature and is a first-order transition.

LJ crystals compared with the Morse system in Ref.\textsuperscript{50} were shown to melt via the third scenario at low temperatures and two continuous BKT transitions at high. This agrees with Ref.\textsuperscript{50} but contradicts Refs.\textsuperscript{14,24}. The BKTHNY scenario at high temperatures was questioned because of seeming disappearance of the Mayer-Wood loop (an analog of the Van-der-Waals loop in the 3D case). For soft Morse interactions, the third melting scenario
crystal melting was examined (at some points) for large systems with \( N = 256^2 \) and \( 512^2 \) particles. The phase diagram was obtained using the dependence of pressure on density (the equation of state) along the isotherms, analysis of the radial distribution functions, orientational and translational order parameters, and the corresponding correlation functions.

B. The method of phase identification

The condensate-gas binodals were obtained using the method of phase identification, proposed in Ref.[87]. The method allows obtaining a binodal in the coordinates density-temperature using analysis of Voronoi cells in the system and, in particular, in terms of the following order parameter[89,97]

\[
\lambda_i = \frac{1}{N_{ni}} + \frac{1}{1} \left( \sigma_i + \sum_{j=1}^{N_{ni}} \sigma_j \right),
\]

\[
\sigma_i = \frac{1}{a_i N_{ni}} \sum_{j<k}^{N_{ni}} (r_{ij} - r_{ik})^2 / 2, \quad r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|,
\]

where \( \mathbf{r}_i \) is the radius-vector of the \( i \)-th particle, \( N_{ni} \) is the number of its neighboring cells, \( a_i = \sqrt{S_i / \pi} \), \( S_i \) is the area of a corresponding Voronoi cell. The scalar \( \lambda^2 \)-field has small values for condensed (liquid and solid) phases, and becomes large at the interface gas-condensate and in gaseous state. Then, analysis of corresponding statistics of Voronoi cells allows obtaining densities \( n_c \) and \( n_g \) of condensate and gas, respectively (see Ref.[87] for details).

To apply the method, additional simulations of a small system with \( N = 3.6 \times 10^3 \) particles under the same \( NVT \) conditions (as we explained above), from \( T_{start} \) to \( T_{stop} \), with step \( T_{step} \) were conducted where each step included \( 6 \times 10^6 \) time-steps with dimensionless time-step \( \Delta t = 5 \times 10^{-4} \) (see the parameters in Table I). At each temperature, we performed phase identification using \( 10^2 \) simulation frames.

This method of phase identification becomes unsuitable near the critical point, where the condensed and

![Generalised LJ potentials with different attraction indices](image-url)

FIG. 1. Generalised LJ potentials with different attraction indices: The solid lines correspond to fixed repulsion with \( n = 12 \) and different indices \( m = 3, 6, 9, \) and 11, illustrating the transition from long- to short-range attractive interactions. The values of cutoff radii \( r_c \) (used for calculations of the equation of state) decrease as shown for each \( m \).

\[ \text{TABLE I. Simulation parameters for potentials LJ12-m used for calculations in the phase identification method, where } a = \rho^{-1/2} \]

| L-Jn-m | \( \rho \) | \( r_c \) | \( T_{start} \) | \( T_{stop} \) | \( T_{step} \) |
|--------|------|------|---------------|---------------|---------------|
| LJ12-3 | 0.3  | 7.5a | 0.7           | 3.05          | 0.06          |
| LJ12-4 | 0.4  | 7.5a | 0.1           | 2.0           | 0.03          |
| LJ12-5 | 0.4  | 7.5a | 0.1           | 1.5           | 0.02          |
| LJ12-6 | 0.4  | 7.5a | 0.1           | 1.5           | 0.02          |
| LJ12-7 | 0.4  | 7.5a | 0.454         | 0.503         | 0.003         |
| LJ12-8 | 0.4  | 7.5a | 0.2           | 0.4           | 0.003         |
| LJ12-9 | 0.4  | 7.5a | 0.14          | 0.3           | 0.002         |
| LJ12-10| 0.4  | 5.0a | 0.09          | 0.151         | 0.001         |
| LJ12-11| 0.5  | 5.0a | 0.025         | 0.076         | 0.001         |

\[ \text{TABLE II. The temperatures and densities in the critical and triple points obtained using the phase identification method} \]

| L-Jn-m | \( T_{CP} \) | \( \rho_{CP} \) | \( T_{TP} \) | \( \rho_{TP} \) |
|--------|---------------|---------------|---------------|---------------|
| LJ12-3 | 1.442         | 0.366         | 0.377         | 1.055         |
| LJ12-4 | 0.748         | 0.453         | 0.455         | 1.042         |
| LJ12-5 | 0.606         | 0.466         | 0.408         | 1.017         |
| LJ12-6 | 0.510         | 0.485         | 0.390         | 1.012         |
| LJ12-7 | 0.480         | 0.486         | 0.399         | 1.015         |
| LJ12-8 | 0.436         | 0.509         | 0.390         | 1.016         |
| LJ12-9 | 0.429         | 0.516         | 0.393         | 1.029         |
| LJ12-10| 0.410         | 0.544         | 0.386         | 0.996         |
| LJ12-11| 0.4053        | 0.550         | 0.3844        | 1.0478        |

We considered cases with fixed repulsion branch \( n = 12 \) and different attraction, from long-range isotropic dipolar attraction with \( m = 3 \) to short-range almost sticky-spheres-like attraction with \( m = 11 \). Examples of the potentials with \( m = 3, 6, 9, \) and 11 are given in Fig. 1. A case similar to usual LJ interaction corresponds to \( n = 12 \) and \( m = 6 \).

The molecular dynamics (MD) simulations were performed for \( N = 2 \times 10^4 \) particles using LAMMPS in the canonical \((NVT)\) ensemble in a wide range of densities and temperatures, from \( T = 0.3 \) to \( T = 50.0 \), using \( 10^8 \) steps with time step \( dt = 10^{-3} \) (in dimensionless units of time normalized to \( \sigma^2 / \epsilon \)). The value of potential energy within cutoff radius \( r_c \) was \( |U(r_c)| < 5 \times 10^{-4} \); it was \( U(r_c) = -4 \times 10^{-4} \) for \( m = 3 \), \( U(r_c) = -3.4 \times 10^{-4} \) for \( m = 6 \), \( U(r_c) = -2 \times 10^{-4} \) for \( m = 9 \), \( U(r_c) = -3.2 \times 10^{-4} \) for \( m = 11 \). To determine accurately the boundaries of two-phase areas, and \( \epsilon \), respectively, and considered the particles of equal mass \( m = 1 \).

and density \( \rho \) using 10 to 4 iterations of the equation of state) decrease as shown for each \( m \).
gaseous phases cannot be distinguished. However, one can obtain the values of critical density \(n_{\text{CP}}\) and temperature \(T_{\text{CP}}\) using the following approximation of the binodal (the results are provided in Table I):

\[
n_{c} - n_{g} \simeq A\tau^{\beta}, \quad n_{c} + n_{g} \simeq a\tau + 2n_{\text{CP}},
\]

(3)

where \(\tau = T_{\text{CP}} - T_{-}\) is reduced temperature, \(\beta\) is a critical index, \(A\) and \(a\) are the free parameters of the model. Critical index \(\beta\) is related to the universality class of the system and is determined by the range of attraction\(^{[3]}\). In 2D systems with dipolar isotropic attraction, \(\beta = 1/2\) (mean-field critical behavior), whereas in the case of shorter-range attraction, at \(m > 3\), \(\beta = 1/8\) corresponds to 2D Ising behavior\(^{[8]}\).

C. Order parameters

For analysis of the phase transition scenarios, we used orientational and translational correlation functions. The orientational correlation function (OCF) of the global orientational order parameter is calculated as:

\[
G_{6}(r) = \frac{\langle \Psi_{6}(r)\Psi_{6}^{*}(0) \rangle}{g(r)}, \quad \Psi_{6} = \frac{1}{N} \left\langle \sum_{ij} \psi_{6}(r_{ij}) \right\rangle,
\]

(4)

where the averaging for \(G_{6}\) is performed over all particles in the system, \(\psi_{6} = 1/n(i) \sum_{j} e^{i\theta_{ij}}\), \(\theta_{ij}\) is the angle of the vector between particles \(i\) and \(j\) with respect to the reference axis, and the sum over \(j\) is counting the \(n(i)\) nearest-neighbors of \(i\), obtained from the Voronoi construction, \(g(r) = \langle \delta(r_{ij})\delta(r_{ij}) \rangle\) is an isotropic pair distribution function (here, \(r_{ij}\) is the position vector of particle \(i\), and \(r = |r_{i} - r_{j}|\)). In the hexatic phase, \(G_{6}(r)\) behaves at large distances like \(G_{6}(r) \propto r^{-\eta_{6}}\) with \(\eta_{6} \leq 1/3^{[17]}\).

The translational correlation function (TCF) is

\[
G_{t}(r) = \frac{\langle \exp(ia(r_{i} - r_{j})) \rangle}{g(r)},
\]

(5)

where \(a\) is the reciprocal-lattice vector of the first shell of the crystal lattice. In the solid phase, \(G_{t}(r)\) behaves at large distances like \(G_{t}(r) \propto r^{-\eta_{t}}\) with \(\eta_{t} \leq 1/3^{[17]}\).

In the hexatic phase and isotropic liquid, \(G_{t}\) decays exponentially.

III. RESULTS AND DISCUSSION

A. The equations of state and phase diagrams

The equations of state (isotherms) for all considered systems behave in a similar manner and have peculiarities that, depending on the temperature and density, are attributed to gas-liquid transition or crystal melting, respectively. This is shown in Fig. 2(a): Here, at isotherm \(T = 0.45\), one can see a wide loop peculiar to gas-liquid transition and a narrow loop related to crystal melting, whereas only one loop related to crystal melting is seen above the gas-liquid critical point at \(T = 1.0\). Below the triple point, at \(T = 0.3\), there is only one wide loop corresponding to gas-crystal transition.

FIG. 2. The equation of state for the 2D LJ system: (a) The isotherms of the system with \(m = 6\) below \((T = 0.3)\) and above \((T = 0.45)\) the triple point and above the critical point at \(T = 1.0\). (b) Isotherm \(T = 0.45\) gas-liquid and isotherm \(T = 0.3\) gas-crystal at low densities. (c) Isotherm \(T = 0.45\) gas-liquid and isotherm \(T = 0.3\) gas-crystal at high densities.

FIG. 3. The isotherms of LJ12-3 system in \(P - V\) coordinates. The gas-liquid transition boundary is obtained using Maxwell’s construction at different temperatures and is shown with the black dashdotted line.
The binodals gas-liquid were calculated using Maxwell’s construction on the isotherms in the $P - V$ coordinates (an example is shown in Fig. 3 for the system with $m = 3$), as well as with the phase identification method. The results for the binodal condensate-gas obtained from the phase identification method and the equation of state are provided in Fig. 4(a). Here, the colored circles denote the densities of gas, condensate, and their average for each potential we considered. The grey solid lines show the regions of the data wherein we used the approximation (3) to obtain data about the critical point. The grey dashed lines show the extrapolation of the phase diagram to the critical points gas-liquid, depicted with colored stars (the corresponding densities and temperatures are given in Table II).

We observed that the drop in the attraction range reduces the critical temperature, as well as the ratio between temperatures of the critical and triple points, as shown in Fig. 4(b) and the corresponding inset (based on the data in Table II). With an increase in $m$ (short-range attraction), the two-phase area becomes narrower towards lower densities and the ratio between the critical and triple temperatures becomes closer to unity, as shown in Fig. 4(b). For LJ interaction ($m = 6$), the critical temperature we obtained is $T_c = (0.51 \ldots 0.52)$ (depending on the method of evaluation), which agrees well with the previous results $T_c = 0.515 \pm 0.002$ for the LJ potential reported in Ref. 13.

At high temperatures, the effect of attraction should vanish, and only the repulsive branch of potential $[1]$ should play a more significant role. Indeed, analyzing the melting scenarios of triangular crystals at high temperatures (and high densities), we observed that LJ12-m systems demonstrated the same melting scenarios as soft disks repulsive potential $1/r^{12}$ (the third melting scenario).

The Mayer-Wood loop was observed in all considered systems at high temperatures, proving first-order transition. However, to determine an appropriate melting scenario, we compared the stability limits of the crystal and the hexatic phases with the boundaries of the Mayer-Wood loop. The stability limits of the hexatic and crystal phases were derived from asymptotic behavior of the correlation functions of the orientational and translational order parameters, respectively. An example of evolution of the correlation functions on the isotherm of the LJ system at $T = 3.0$ is shown in Fig. 5.

In Fig. 5(a), the equation of state is shown at $T = 3.0$ (obtained by averaging over 20 independent replicas) for the LJ system consisting of $N = 512^2$ particles. One can see the clearly defined Mayer-Wood loop, inherent in the first-order transitions. Analyzing the correlation functions in Figs. 5(b,d), we conclude that the loop corresponds to the two-phase hexatic-liquid area, whereas the melting scenario is the third, with a continuous BKT transition from crystal to hexatic and a first-order transition from hexatic to liquid. Here, the hexatic phase becomes unstable at $\rho_{hex-liquid} = 1.014$ (Fig. 5(b)), inside the loop, whereas the crystal becomes unstable at $\rho_{sol-hex} = 1.037$ (Fig. 5(c)) getting far out of the loop. The obtained results agree well with the melting scenario for repulsive disks $1/r^{12}$ (reported in Refs. 14,15, but do not exhibit two continuous BKT transitions in the LJ system at high temperatures. The obtained results agree well with the melting scenario for repulsive disks $1/r^{12}$ (reported in Refs. 14,15, but do not exhibit two continuous BKT transitions in the LJ system at high temperatures.

![Figure 4](image-url)
FIG. 5. **Evolution of correlation functions on an isotherm:** (a) The isotherm $T = 3.0$ for LJ system consisting of $N = 512^2$, obtained by averaging over 20 independent replicas. (b) and (c) The OCF and TCF for the same system at different densities.

All triangular crystals, we studied, were found to melt at high temperatures via the third scenario, irrespective to the attraction index $m$. The melting lines in this region of the phase diagram are shifted to low densities with an increase in $m$ and behave similarly to a system of soft disks $1/r^{12}$, as shown in Fig. 6.

However, with a decrease in melting temperature, the balance of the effects provided by the repulsive and attractive branches is changed. As a result, we observed that, at low temperatures, the melting scenario changes from the third one to a first-order transition ($T = 0.6$) to the third scenario ($T = 0.7$). The arrows show the stability limits of the hexatic phase, $G_6$, are obtained using the OCF, and the stability limits of the crystalline phase, $G_t$, are obtained with TCF, which become caught by the loop with a decrease in temperature.

**FIG. 6. The third melting scenario of the triangular crystals at high temperatures and densities:** The solid lines are the boundaries of the Mayer-Wood loop corresponding to the two-phase hexatic-liquid area. The dashed lines are the boundaries of BKT transition from the crystal to hexatic phase. The results are provided for the cases $m = 3, 6, 9$, and 11, as labeled in the figure.

**FIG. 7. The change in the melting scenario for the case $m = 9$:** The melting scenario changes from a first-order transition ($T = 0.6$) to the third scenario ($T = 0.7$). The arrows show the stability limits of the hexatic phase, $G_6$, are obtained using the OCF, and the stability limits of the crystalline phase, $G_t$, are obtained with TCF, which become caught by the loop with a decrease in temperature.

B. **The results for isotropic dipolar attraction**

In the case of LJ12-3 potential, the crystal was found to melt at low temperatures according to the third scenario. However, the hexatic phase was discovered to be preserved up to triple point temperature $T_t$, where it coexists with both liquid and gaseous phases, as given in Fig. 8.

This unexpected result is explained using the Gibbs rule: Due to the reduced spatial dimension and since melting represents a two-stage process, we obtain a couple of points where three phases may exist simul-
Pressure, $P$

-1.0
-0.5
0.0
0.5
1.0
1.5
2.0

Density, $\rho$

0.0
0.5
1.0
1.5
2.0

FIG. 8. The cascades of phase transitions: Isotherm $T = 0.6 > T_1$ illustrates the cascade of a first-order gas-liquid transition, first-order liquid-hexatic transition, and a continuous BKT crystal-hexatic transition. At $T = 0.57 < T_1$, only a first-order gas-hexatic transition and a continuous BKT crystal-hexatic transition are seen. Detailed behavior of the isotherms at high densities are shown in the inset. At negative pressures and $T = 0.57 < T_1$, one can see a loop related to the first-order transition gas-hexatic (in the metastable area), while a continuous BKT crystal-hexatic transition still occurs at positive pressure. The arrows show the limits of stability of the hexatic phase $G_6$ and of the crystal $G_t$, obtained using OCF and TCF analysis, respectively.

At high densities in the vicinity of the crystalline phase, additional modulations of the loops may be interpreted as two-stage melting of the metastable crystal appearing in the equation of state. In this case, phase identification was performed using analysis of the radial distribution functions, behavior of the orientational and translational order parameters, and their correlation functions. We observed a transition of the metastable crystal to the hexatic phase through a continuous BKT transition with a subsequent first-order transition from hexatic to gas. With a decrease in temperature, the region of the hexatic phase narrows on the phase diagram, and disappears completely at $T = 0.45$, which leads to one first-order crystal-gas transition, as shown in Fig. 10.

For the case of isotropic dipolar attraction $m = 3$, the phase diagrams in different coordinates are presented in Figs. 11(a,b). Here, the lines of phase coexistence, critical, and triple points are shown in Fig. 11(a). In the density-temperature plane, a two-stage crystal-gas transition occurs in the metastable area of the hexatic phase and crystal at $T < T_{12}$, see Fig. 11(b). In Fig. 11(c) an enlargement of the phase diagram is represented the behavior of different domain boundaries on the phase diagram near triple points $T_1$ and $T_{12}$. We note in conclusion that, with an increase in the number of particles in the system, the loops corresponding to gas-crystal transition should flatten. This leads to the disappearance of the metastable area of the crystal and to the first-order gas-crystal transition, without the modulation of
the equation of state mentioned above.

IV. CONCLUSIONS

In this work, we studied the evolution of the phase diagrams and melting scenarios of two-dimensional systems of particles interacting via generalized LJ potential with a different attraction range, whereas the repulsion branch was fixed. Gas-liquid transition was studied using analysis of the equation of state and the phase identification method. The results obtained by the two methods stand in good agreement indicating their consistency. The drop in the attraction range reduces the gas-liquid coexistence region and temperatures of the critical and triple points.

Melting at high temperatures (and high densities) is found to behave like a system of soft disks $1/r^2$, via the third scenario. However, at low melting temperatures, a change in the melting scenario was identified from the third scenario to a first-order transition (without the hexatic phase) in the systems with $m = 6, 9, 11$. The temperature of the change in the scenarios is shifted toward lower temperatures with an increase in the attraction range (corresponding to the decrease in $m$). Analysis of the case $m = 9$ (LJ12-9), very close to that studied in Ref.$^{60}$ demonstrated that for short-range attraction in complex solvents we should witness the third melting scenario.

The largest region of gas-liquid coexistence was observed in the phase diagram in the $\rho - T$ coordinates in the case of $m = 3$. Due to soft long-range isotropic dipolar attraction, we unexpectedly saw two triple points at $T_{11}$ and $T_{12}$, corresponding to hexatic-liquid-gas and to crystal-hexatic-gas equilibrium, respectively. On the isotherms in the interval between two triple points $T_{12}$ and $T_{11}$, we observed a continuous BKT transition from crystal to hexatic phase and a first-order transition from hexatic to gas. At the crystal-gas sublimation line, a first-order transition from crystal to gas has been identified.

The main conclusions related to the scenario of phase transitions in a system with dipolar attraction can be tested in future experiments with colloidal systems, wherein the tunable long-range dipolar attraction can be created with rotating magnetic or electric fields. A nontrivial question here is related to the role of three-body forces, inherent in atomic materials and tunable colloids. LJ-like interactions can be created with magic holographs of rotating electric or magnetic fields.$^{75}$ However, three-body interactions in this case behave as $\propto 1/r^6$, with the same asymptotics as pairwise potential. Due to this, the scenario of melting can change, and we leave the corresponding study to future work.

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E.N.T., Y.D.F., and E.A.G. performed MD simulations to obtain phase diagrams, N.A.D., P.A.L., and N.P.K. obtained condensate-gas binodals with phase identification method, E.N.T., V.N.R., E.E.T., N.P.K., and S.O.Y. analysed and discussed the results, E.N.T., V.N.R., and S.O.Y. wrote the manuscript, V.N.R. and S.O.Y. conceived and directed the study.

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FIG. 11. The phase diagram of the LJ12-3 system: (a) The phase diagram in the \((P - T)\) coordinates. (b) The phase diagram in the \((\rho - T)\) coordinates. \(T_{CP}\) is a gas-liquid critical point, \(T_{t1}\) is a hexatic-liquid-gas triple point, and \(T_{t2}\) is a crystal-hexatic-gas triple point. Gas, liquid, hexatic phase and crystal are denoted as G, L, Hex, and S, respectively. The regions of their coexistence are marked as G+L, G+Hex, and G+S. The solid and dashed lines correspond to a first-order transition and to continuous BKT crystal-hexatic phase transition, respectively. The two-stage crystal-gas transition in the metastable area of the hexatic phase and crystal at \(T < T_{t2}\) are denoted with open symbols. (c) The enlarged region of the phase diagram in the area of triple points \(T_{t1}\) and \(T_{t2}\).