REVIEWS OF TOPICAL PROBLEMS

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Berezinskii–Kosterlitz–Thouless transition and two-dimensional melting*

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Abstract. The main aspects of the theory of phase transitions in two-dimensional degenerate systems (Berezinskii-Kosterlitz-Thouless, or BKT, transitions) are reviewed in detail, including the transition mechanism, the renormalization group as a tool for describing the transition, and how the transition scenario can possibly depend on the core energy of topological defects (in particular, in thin superconducting films). Various melting scenarios in two-dimensional systems are analyzed, and the current status of actual experiments and computer simulations in the field is examined. Whereas in three dimensions melting always occurs as a single first-order transition, in two dimensions, as shown by Halperin, Nelson, and Young, melting via two continuous BKT transitions with an intermediate hexatic phase characterized by quasi-long-range orientational order is possible. But there is also a possibility for a first-order phase transition to occur. Recently, one further melting scenario, different from that occurring in the Berezinskii-Kosterlitz-Thouless-Halperin-Nelson-Young theory, has been proposed, according to which a solid can melt in two stages: a continuous BKT-type solid-hexatic transition and then a first-order hexatic-phase-isotropic-liquid phase transition. Particular attention is given to the melting scenario as a function of the potential shape and to the random pinning effect on two-dimensional melting. In particular, it is shown that random pinning can

V N Ryzhov, E E Tareyeva, Yu D Fomin, E N Tsiok Vereshchagin Institute for High Pressure Physics, Russian Academy of Sciences, Kaluzhskoe shosse 14, 108840 Troitsk, Moscow, Russian Federation E-mail: ryzhov@hppi.troitsk.ru, etare@ms2.inr.ac.ru, fomin314@mail.ru, elena.tsiok@gmail.com Received 15 May 2017, revised 23 June 2017

Uspekhi Fizicheskikh Nauk **187** (11) 921–951 (2017) DOI: https://doi.org/10.3367/UFNr.2017.06.038161 Translated by E N Ragozin; edited by A M Semikhatov alter the melting scenario fundamentally in the case of a firstorder transition. Also considered is the melting of systems with potentials having a negative curvature in the repulsion region potentials that are successfully used in describing the anomalous properties of water in two dimensions.

Keywords: two-dimensional systems, Berezinskii–Kosterlitz– Thouless transition, superfluid films, superconducting films, *XY* model, two-dimensional crystals, topological defects, vortices, dislocations, disclinations, hexatic phase, two-dimensional melting, Berezinskii–Kosterlitz–Thouless–Halperin–Nelson–Young theory, first-order transition

1. Introduction

On October 4, 2016, the names of the laureates of the 2016 Nobel Prize in physics were announced in Stockholm: these were the British physicists David Thouless, now at the University of Washington in Seattle (USA), and Duncan Haldane of Princeton University (USA), as well as John Michael Kosterlitz of Brown University in Providence (USA), "for theoretical discoveries of topological phase transitions and topological phases of matter," according to the Nobel citation. Duncan Haldane is undoubtedly an outstanding theoretical physicist, recognized for his work on the topological states in one-dimensional magnetic chains and the fractional Hall effect, but in this review we restrict ourselves to a discussion of the properties of the Kosterlitz– Thouless transition (to be more precise, the Berezinskii– Kosterlitz–Thouless transition).

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Prior to turning to the description of the physical aspects and applications of the theory developed by the laureates, it is necessary to enlarge on one issue that arises for anyone who is familiar, at least vaguely, with the history of this discovery. In the English-language scientific literature, the term "Kosterlitz–Thouless transition" is commonly used, while Russian scientists most often speak about the Berezinskii–Kosterlitz– Thouless (BKT) phase transition.

It is hard to overestimate the role of the untimely deceased talented Soviet physicist Vadim L'vovich Berezinskii in the development of the theory of phase transitions in degenerate planar systems. Berezinskii was the first to formulate the fundamentals of the theory [1, 2] that was awarded the Nobel Prize in 2016. It is pertinent to note that the basic paper by Kosterlitz and Thouless [3] contains due references to both Berezinskii's papers on this subject and appropriate commentaries. Furthermore, in his 2016 review [4] expressively entitled "Kosterlitz-Thouless physics: a review of key issues," Kosterlitz wrote that he and Thouless felt disappointment when they learned about the earlier work by Berezinskii. However, Kosterlitz noted there that he and Thouless did not know Russian and were not familiar with Berezinskii's work. We note, however, that the Journal of Experimental and Theoretical Physics (JETP), where Berezinskii's paper was published, was translated into English on a regular basis at that time (see, e.g., Ref. [5]).

Phase transitions are among the most frequently occurring and interesting effects, which are encountered in everyday life as well as in basic research and technological applications. A theory that proved to be capable of describing the key aspects of the physics of phase transitions was proposed by Landau [6] in 1937. The basic point of Landau's theory is his proposed notion of the order parameter—a quantity that is equal to zero at temperatures above the transition temperature (in the disordered phase) and takes nonzero values in the ordered phase. The order parameter characterizes symmetry breaking that occurs in phase transitions.

According to the standard classification, there are two types of phase transitions: of the first order, where the order parameter experiences a discontinuity, and continuous (often referred to as second-order transitions), where the order parameter changes continuously. The simplest example of the order parameter is magnetization (the average value of the magnetic moment) in a ferromagnetic material. Qualitatively, the transition in a magnet can be represented as follows: at a high temperature, magnetic moments rotate freely and there is no preferred direction in the system, which is therefore isotropic. As the temperature decreases, however, at some critical temperature $T_{\rm c}$, a nonzero value of magnetization (of the order parameter) spontaneously appears in the system, i.e., a phase transition to the ferromagnetic state occurs. In this case, a preferred direction appears, which coincides with the direction of the magnetization vector, and the system ceases to be isotropic.

Landau's theory did not take thermal fluctuations of the order parameter into account, but nevertheless provided a quite satisfactory description of experimental facts. The most brilliant achievement of this theory was the phenomenological description of superconductivity, for which A A Abrikosov and V L Ginzburg were awarded the 2003 Nobel Prize. At the same time, by the 1960s it became clear that the inclusion of fluctuations is critical for correctly describing the behavior of a system in the vicinity of a second-order phase transition.

This resulted in the construction of the fluctuation theory of phase transitions (A Z Patashinskii, V L Pokrovskii, L Kadanoff, M Fisher, K Wilson) (see, e.g., Refs [7–14]), which brought Wilson the Nobel Prize in 1982.

The above and other authors called attention to the role of the dimensionality of space in which the transition occurs in the description of its properties. In particular, as shown by Peierls and Landau, and later by Bogoliubov, Mermin, and Wagner, in two-dimensional systems with continuous order parameter symmetry (the Heisenberg magnet, the plane rotor (or XY) model, superfluid and superconducting systems, as well as two-dimensional crystal lattices), thermal fluctuations destroy the long-range order, which means that a nonzero value of the order parameter extends to the entire system. Hence, it was concluded that a phase transition in such systems is possible only at a zero temperature. At the same time, experimental works on superfluidity in thin liquid helium-4 films appeared [15-21], as did several investigations based on computer simulations of hard disks [22-26] and numerical techniques applied to magnetic systems [27-29], which were at variance with the above-mentioned conclusion.

It was Berezinskii, Kosterlitz, and Thouless [1-3, 30, 31] who clarified the matter. Berezinskii [2] was the first to show that a thin liquid helium film, even without a long-range order, exhibits superfluidity at low temperatures. Twodimensional crystals, although exhibiting no long-range translation order, have a finite shear modulus and are therefore solid. Two-dimensional magnets are resistant to nonuniform rotation of spins. Berezinskii recognized that these phenomena are common in nature and devised the term 'transverse rigidity' for them, which is now commonly used in the literature. For systems with transverse rigidity, Berezinskii showed that the two-point correlation functions that describe the mutual effect of order parameters exhibit a slow power-law decay with distance, with the power depending on the interaction parameters and the temperature. We recall that in the presence of long-range order, a similar correlation function tends to a nonzero limit as the distance between the points tends to infinity, while in the high-temperature disordered phase, correlations decay exponentially fast.

The new phase, sometimes referred to as the Berezinskii phase, is fundamentally different from what can be observed in three dimensions. In view of the slow decay of correlations, this phase is commonly said to have a quasi-longrange order. Similar results were later obtained by Kosterlitz and Thouless [3, 30]. Furthermore, they corrected an error made by Berezinskii, who mistakenly believed that a quasilong-range order can exist in a two-dimensional Heisenberg magnet, i.e., in a system with three-component magnetic moments.

Because the correlations in the low- and high-temperature phases obey different decay laws that do not match smoothly, it became clear that there should be a phase transition between them. Berezinskii discovered the important role of topological effects in the transition — vortices in a superfluid helium film, dislocations in a two-dimensional crystal, and vortex configurations in a two-dimensional magnet with twocomponent magnetic moments (*XY* model) — and provided a qualitative explanation for the transition mechanism. At a low temperature, defects couple into pairs, which do not break the quasi-long-range order. However, as the temperature increases, the pairs dissociate giving rise to free defects, which transform the quasi-long-range order into a disordered phase with an exponentially fast correlation decay. A method for calculating the transition temperature was developed in subsequent work by Kosterlitz and Thouless [3, 30, 31].

The theory of transitions in two-dimensional degenerate systems developed by Berezinskii, Kosterlitz, and Thouless has played an outstanding role in the study of the physics of two-dimensional melting. Despite the almost 40-year-long history of the problem, so far there is no theory that consistently describes the melting of two-dimensional systems from the microscopic standpoint. The problem of twodimensional melting is among the oldest unsolved problems of condensed matter physics. Although a wealth of publications is concerned with this subject, contradictions relating to the description of melting in two dimensions persist and even multiply. Unlike melting in the three-dimensional case, which always occurs due to conventional first-order transitions [32], two-dimensional melting can be described by several proposed scenarios. The main reason for this difference is a dramatic increase in fluctuations in passing from two to three dimensions. Peierls, Landau, and, more recently, based on the Bogoliubov $1/q^2$ theorem [33–35], Mermin [36] showed that the long-range crystalline (translational) order cannot exist in two dimensions owing to thermodynamic fluctuations and transforms into a quasi-long-range order characterized by a slow decay of order parameter correlations. On the other hand, true long-range orientational ordering (the order in the orientations of 'bonds' connecting a molecule to its nearest neighbors) does take place in two dimensions, as was first noted by Mermin [36]. In this case, an ordinary isotropic liquid exists at high temperatures.

Even in their original work [3], Kosterlitz and Thouless noted that a two-dimensional crystal should melt by dissociation of dislocation pairs, which are topological defects in this case. In the presence of the quasi-long-range translational order, these effects are well defined. Besides the quasi-longrange translational order, long-range orientational order exists in a two-dimensional crystal, i.e., the order in the directions of the vectors connecting a particle to its nearest neighbors, and therefore, as later noted by Halperin and Nelson [37, 38] (see also Ref. [39]), a liquid turns out to be anisotropic in a state above the point of dislocation pair dissociation. The authors of Refs [37, 38] noted that dislocation pair dissociation does not destroy the long-range orientational order but transforms it into a quasi-long-range order. The resultant new phase received the name 'hexatic' by analogy with liquid crystals. In the hexatic phase, there are free dislocations, and therefore its shear modulus is equal to zero, which means that we here deal with a liquid with elements of ordering.

We note that a dislocation can be represented as a coupled pair of two disclinations. The hexatic phase transforms into an ordinary isotropic liquid as a result of the subsequent BKT transition via dissociation of disclination pairs. The presented theory bears the name Berezinskii–Kosterlitz–Thouless– Halperin–Nelson–Young (BKTHNY) theory. In the framework of this theory, a two-dimensional crystal should melt by means of two continuous BKT transitions with an intermediate hexatic phase (we recall that melting in the threedimensional case is always a first-order transition). As was shown later, a first-order transition is also possible for a low dislocation core energy.

The BKTHNY theory seems to be highly attractive and universal, and in a sense one may hypothesize that all twodimensional crystal should melt in the framework of this scenario. However, some of its aspects are debatable. In the framework of this theory, for instance, there is no way of calculating the energy of a topological defect core or the energy of the effective interaction between disclinations in the hexatic phase. The BKTHNY theory gave rise to a wealth of publications, both experimental and those reliant on computer simulations, some of which are described below.

Presently, it is believed that the melting scenario of a twodimensional system is radically dependent on the kind of interparticle interaction. In particular, it was shown that the BKTHNY theory is applicable to systems with a long-range interaction. For systems with short-range potentials, the melting can also occur via two transitions with an intermediate hexatic phase; in this case, however, the crystalhexatic phase transition proceeds in accordance with the BKT theory, while the hexatic phase transforms into an isotropic liquid by a first-order transition (see the discussion in Sections 3.7 and 4).

There are numerous books and reviews that discuss many aspects and applications of the BKT theory. First of all, we note book [40] reproducing Berezinskii's thesis. Book [41], which was published to the 40th anniversary of the first papers by Kosterlitz and Thouless, is a collection of papers concerned with different aspects of BKT theory applications to various systems (see the review of this book in Ref. [42]). As mentioned above, published in 2016 was the review by Kosterlitz [4], which not only considered numerous aspects and applications of the BKT theory but also contained interesting remarks relating to the construction of this theory.

In this review, we outline the basic ideas underlying the BKT theory, including issues that were not treated at length in the publications cited above. In doing so, we place emphasis on the modern state of the theory and experiment in the physics of two-dimensional melting.

2. Berezinskii–Kosterlitz–Thouless theory

2.1 Berezinskii–Kosterlitz–Thouless transition in the *XY* model and in superfluid films

The BKTHNY theory is underlain by the mechanism of quasi-long-range order breaking in two-dimensional systems with a continuous symmetry group, which was proposed by Berezinskii [1, 2] and by Kosterlitz and Thouless [3, 31]. Examples of such systems are provided by two-dimensional superconductors and superfluid liquids with the order parameter of the form $\psi = \sqrt{\rho_s} \exp(i\theta)$, where ρ_s is the superfluid component density and θ is the phase of the order parameter, and by the classical *XY* model described by the Hamiltonian

$$H = -\frac{J}{2} \sum_{\langle i \neq j \rangle} \mathbf{S}_i \mathbf{S}_j \simeq \frac{J}{2} \int \mathrm{d}^2 r \left(\nabla \omega \right)^2, \tag{1}$$

where J is the exchange integral, S_i and S_i are the classical magnetization vectors, and ω is the angle between vectors S_i and S_j (*i* and *j* are nearest neighbors).

At low temperatures, the behavior of the system is governed by Gaussian fluctuations. We use the mean value theorem for Gauss-distributed quantities to find

$$\langle \mathbf{S}(\mathbf{r}) \, \mathbf{S}(\mathbf{r}_0) \rangle \\ = \langle \exp\left[i\left(\omega(\mathbf{r}) - \omega(\mathbf{r}_0)\right)\right] \rangle \propto \left(\frac{|\mathbf{r} - \mathbf{r}_0|}{a_0}\right)^{-k_{\rm B}T/(2\pi J)}, \quad (2)$$

where a_0 is the lattice constant. Therefore, the system has a quasi-long-range order characterized by power-law correlation decay, $\langle \mathbf{S}(\mathbf{r}) \mathbf{S}(\mathbf{r}_0) \rangle \propto r^{-\eta}$, while at high temperatures the correlations decay exponentially, $\langle \mathbf{S}(\mathbf{r}) \mathbf{S}(\mathbf{r}_0) \rangle \propto \exp(-r/\xi)$ (see, e.g., Ref. [14]). The mechanism of quasi-long-range order breaking was proposed in the works by Berezinskii, Kosterlitz, and Thouless mentioned above. They showed that quasi-long-range order breaking in a system results from the formation of free topological defects — vortices described by the equation

$$\frac{\delta H}{\delta \omega} = J \nabla^2 \omega = 0, \qquad (3)$$

whose solution is of the form

$$\omega = q \arctan \frac{y}{x}, \quad \mathbf{v}_q = \nabla \omega = \frac{q}{r} \,\mathbf{e}_{\varphi} \,.$$
(4)

Here, $q = \pm 1, \pm 2, ...$ is the topological vortex charge and \mathbf{e}_{φ} is the unit vector in a polar coordinate system with the origin at the vortex center. Then $\oint (\nabla \omega) dl = 2\pi q$, where the integral is taken along the contour around the vortex.

A vortex is a topological defect that *cannot* be transformed by continuous rotations into the ground state, wherein all spins point in the same direction. Figure 1 shows two vortices on a square lattice with q = +1 and q = -1. Shown in Fig. 2 is a dipole consisting of a vortex and an antivortex. This configuration can be continuously transformed into the ground state.

The transition temperature can be determined from simple energy considerations: the energy of an individual vortex obtained from Eqn (1) is of the form

$$E_{\rm v} = \frac{J}{2} \int_0^L \frac{2\pi}{r} \, {\rm d}r = J\pi \ln \frac{L}{a} \,, \tag{5}$$

where *L* is the system size. The change in the free energy upon production of a vortex is $F = E_v - TS$, where $S = 2k_B \ln(L/a)$ is the vortex entropy, which is proportional to the area of the system, and k_B is the Boltzmann constant. The quantity $F = (J\pi - 2k_BT) \ln(L/a)$ turns out to be negative for $T \ge T_{BKT} = \pi J/(2k_B)$, and hence the production of a vortex becomes energetically favorable.

As follows from Eqn (2), at $T = T_{\text{BKT}}$, the correlation function has the form $\langle \mathbf{S}(\mathbf{r}) \mathbf{S}(\mathbf{0}) \rangle \propto r^{-1/4}$. Therefore, at the transition point, the correlation function exponent is $\eta = 1/4$.

However, this simple physical picture is not entirely correct because the coupled pairs of oppositely 'charged' vortices do not destroy the quasi-long-range order and have a finite energy (see Fig. 2). Such pairs can exist at low temperatures. The above Hamiltonian of the subsystem of



Figure 1. (a) Positive, q = +1, and (b) negative, q = -1, vortices on a square lattice.



Figure 2. Dipole of positive and negative vortices on a square lattice.

the vortices is equivalent to the Hamiltonian of a twocomponent two-dimensional Coulomb gas [3, 43]:

$$H_{\rm c} = -\pi J \sum_{i < j} q(\mathbf{r}_i) q(\mathbf{r}_j) \ln \frac{|\mathbf{r}_i - \mathbf{r}_j|}{a} + E_{\rm c} \sum_i q^2(\mathbf{r}_i) .$$
(6)

The harmonic approximation used in the derivation of Eqn (6) is invalid for small r, and hence the core energy E_c was introduced to include the contribution made by the small-r domain of the order of the core diameter a. E_c plays the role of the chemical potential of the Coulomb gas.

At the phase transition point, the mean-square distance $\langle r^2 \rangle$ between the vortices that form a dipole becomes infinite:

$$\langle r^2 \rangle \propto \int_a^\infty r^2 \exp\left(-\frac{E(r)}{T}\right) r \,\mathrm{d}r = \int_a^\infty r^{3-1/(2\Delta)} \,\mathrm{d}r \,, \qquad (7)$$

where $\Delta = k_{\rm B}T/(4\pi J)$. Here, formula (6) is used for E(r). Integral (7) diverges at large *r* for $\Delta \ge 1/8$.

A superfluid film is described by a Hamiltonian coinciding in form with Hamiltonian (1), with the substitution $J \rightarrow \hbar^2 \rho_s(T)/m^2$, where *m* is the mass of ⁴He atoms and $\rho_s(T)$ is the superfluid component density. In then follows that $\Delta = k_{\rm B}T/(4\pi J) = k_{\rm B}Tm^2/(4\pi\hbar^2\rho_s(T))$. From the condition $\Delta = 1/8$, it follows that the ratio of the superfluid density to the transition temperature for the superfluid helium film, which was theoretically found by Kosterlitz and Nelson [4] and experimentally confirmed in [45, 46], turns out to be a combination of world constants:

$$\frac{\rho_{\rm s}(T_{\rm BKT})}{T_{\rm BKT}} = \frac{2m^2}{\pi\hbar^2} \,. \tag{8}$$

Interestingly, the BKT phase transition combines the features of jump-like and continuous behaviors: the entropy, the area, and even the heat capacity change continuously, while the transverse rigidity (the superfluid density) jumps to zero.

The BKT transition mechanism [1-3] is the dissociation of a dilute vortex-pair gas. The Coulomb potential screening due to thermally excited pairs must be taken into account here.

The dissociation occurs at the temperature at which the permittivity of the two-dimensional Coulomb gas diverges.

The BKT theory is a renormalization-group treatment of screening effects. The theory predicts a continuous transition from the low-temperature phase with a quasi-long-range order to the high-temperature disordered phase. In this case, the quantity $K = J/(k_BT)$ renormalizes at the transition point T_{BKT} to a universal limit value, which then jumps to zero. The equations describing the renormalization of the parameters of the system in the vicinity of the transition were derived in Ref. [3], but they were found incorrectly, because the approximation was not quite correct. The inaccuracy was corrected by Young [47], resulting in the derivation of renormalization group equations of the presently well-known form [4, 14, 31, 43, 47]

$$\frac{\mathrm{d}y(l)}{\mathrm{d}l} = (2 - \pi K(l, T)) y(l) ,$$

$$\frac{\mathrm{d}K^{-1}(l, T)}{\mathrm{d}l} = 4\pi^3 y^2(l) ,$$
(9)

where $l = \ln r$ and y is the fugacity. The solution of Eqns (9) has been repeatedly discussed (see, e.g., Refs [4, 14, 41, 43]), and we do not discuss it here. We only note that Eqns (9) are valid for $y \ll 1$. Because $y \propto \exp(-E_c/(k_BT))$, it can be inferred that they correspond to the case of high energies of the topological defect core. This is a very important point, and we return to its discussion below. As a result of the solution of system (9), the (y, K^{-1}) plane is divided into three domains. In the first one, $y \to 0$ as $l \to \infty$, while $K^{-1}(l, T)$ tends to a finite renormalized value defined by the initial temperature-dependent values $K_0^{-1}(l, T)$. The transition temperature T_{BKT} is defined as the highest temperature at which the renormalized $K^{-1}(l, T)$ value remains finite as $l \to \infty$. For $T = T_{\text{BKT}}$ and $l \to \infty$, we obtain the relation

$$K(l \to \infty, T_{\rm BKT}) = \frac{J_{\rm r}(l \to \infty, T_{\rm BKT})}{T_{\rm BKT}} = \frac{2}{\pi} , \qquad (10)$$

where J_r is the renormalized value of the exchange integral. It is noteworthy that the transition temperature obtained using the renormalization group method is formally coincident with the temperature calculated above from simple energy considerations, if the coupling constant is replaced with its renormalized value. The physical meaning of renormalization is rather simple: with an increase in $l = \ln r$, the influence of paired vortices vanishes, and the part of the renormalized Hamiltonian that corresponds to topological defects is removed. As a result, a quasi-long-range order sets in within this domain. The two remaining domains of the phase diagram in the $y-K^{-1}$ plane are characterized by both y(l, T) and $K^{-1}(l, T)$ approaching infinity as $l \to \infty$ for any initial values $y_0(l, T)$ and $K_0^{-1}(l, T)$.

At temperatures $T > T_{BKT}$, the correlation function decays exponentially. In this case, the correlation length exponentially tends to infinity as the temperature approaches the transition temperature from above [4, 14, 41, 43]:

$$\xi \propto \exp\left(\frac{\mathrm{const}}{\left|T-T_{\mathrm{BKT}}\right|^{1/2}}\right).$$

Equations (9) were derived by Kosterlitz [31] (see also Young's work [47]) in the framework of the two-dimensional Coulomb gas model. More recently, they were rederived by standard methods of quantum field theory in Refs [49–51] using a representation of the partition function of a twodimensional Coulomb gas in the field theory framework with the Hamiltonian of the sine-Gordon form [43]. Obtained in Ref. [51] was the next approximation in the expansion in the small parameters y and $2 - \pi K(l, T)$.

In a series of studies by Minnhagen et al. [43, 52-64], an attempt was made to go beyond the lowest-order approximation in powers of the fugacity y in the derivation of renormalization group equations. In the framework of the sine-Gordon theory and dielectric formalism, they obtained a system of nonlinear integro-differential equations that led to the same BKT transition point for small y. The behavior of the system in the vicinity of this point corresponds to the results obtained from the standard system (9) and the equations derived in Ref. [51], but the entire phase diagram turns out to be much more complex. In the limit of a low vortex density (of high energy of the topological defect core), the transition is described in the renormalization group framework [31] and is a continuous transition of infinite order. In the high-density case, the vortices can dissociate by a first-order transition, as has been shown, for instance, using renormalization group equations [43, 61, 62] and the Monte Carlo method [63-69]. The first-order transition line terminates at the critical point. The BKT transition line continuously joins the first-order transition line at temperatures somewhat lower than the critical temperature. It turned out that the jump universality (8) is violated in the first-order transition domain and the correlation function exponent $\eta \neq 1/4$.

A first-order transition in a two-dimensional Coulomb gas was also discovered in the framework of the sine-Gordon theory in Refs [70, 71].

Levin and Fisher [48] calculated the phase diagram (Fig. 3) of a two-dimensional Coulomb gas using the Debye–Hückel and Boltzmann–Poisson approaches supplemented with the method described in Ref. [72] [Debye–Hückel–Bjerrum Dipole-Ion-Hard-Core (DHBjDIHC) theory]. As is clear from the phase diagram, a BKT-type transition occurs in the system at low densities, with the formation of coupled states



Figure 3. Phase diagram of a two-dimensional Coulomb gas in temperature–density variables (T^*, ρ^*) . Here, $\rho^* = \rho d^2$, *d* is the ion core diameter, $\rho_1 = \rho_+ + \rho_-$, $T^* = k_B TD/q^2$, *D* is the permittivity of the system, and *q* is the ion charge. Calculations were made in the framework of the DHBjDIHC model [48].

of positive and negative charges. At higher densities, the coupled states dissociate by a first-order transition.

We note that the use of standard methods of classical statistical mechanics, of Mayer diagrams [73] in the first place, turn out to be rather beneficial for describing the behavior of the two-dimensional Coulomb gas [74–77]. In particular, renormalization group equations (10) were derived in [76, 77] using Mayer expansions.

Special mention should be made of the paper by Salzberg and Prager [78]: in considering the behavior of two-dimensional electrolytes—10 years before the publication by Kosterlitz and Thouless [3]—they were the first to find the condition for dissociation of coupled pairs in a two-dimensional Coulomb gas, which coincides with the condition for dissociation of topological defects obtained by Kosterlitz and Thouless a decade later [3, 30]. Unfortunately, this short paper (less than one page long) was never developed further.

2.2 Berezinskii–Kosterlitz–Thouless-type transition in a thin superconducting film (cycle approximation)

The special features of intervortex interactions in a thin superconducting film do not allow describing the dissociation of vortex-antivortex pairs (a BKT-type transition) by adhering to the unambiguous analogy with the XY model or the system of vortices in a thin superfluid film. Applications of the BKT theory to two-dimensional superconducting systems are discussed in detail, for instance, in book [41] and in reviews [4, 43].

In this section, we consider an approach to describing this transition within the cycle approximation used to calculate thermodynamic quantities for a system of vortices with a long-range intervortex interaction.

As mentioned above, Kosterlitz and Thouless [3] proposed a theory for the phase transition in neutral superfluid films in terms of vortex–antivortex pair dissociation. However, it was mistakenly stated in [3] that coupled vortex–antivortex pairs cannot be produced in a thin superconducting film because the intervortex interaction behaves as 1/r in a thin superconducting film at long range, while the BKT transition requires a logarithmic increase in the interaction potential.

The applicability of the BKT theory to superconducting films was first discussed in Ref. [79]. For an infinite superconducting film of thickness *d* and bulk penetration depth $\lambda_B(T)$, Pearl [80] showed that the intervortex interaction energy behaves logarithmically for $r \ll \Lambda(T) = 2\lambda_B(T)/d$ and behaves as 1/r for $r \gg \Lambda$. The quantity Λ can be regarded as the effective penetration depth for the magnetic field perpendicular to the film plane. The BKT transition would be expected to occur when Λ exceeds the film size. This condition can be reached both by decreasing the film thickness and by enhancing the degree of disorder in the system, as was first noted in Ref. [79]. Hence, it can be concluded that the phase transition, in its strict sense, does not exist in a superconducting film because free vortices exist in it for any T > 0.

As shown in Ref. [79], type-II superconducting thin films can have an effective penetration depth of the order of several centimeters, i.e., experimental samples can be smaller in size than Λ . To describe vortices in a charged two-dimensional superfluid liquid in this case, an approximate analogy with a two-dimensional Coulomb gas can be used [43, 79]. Therefore, the authors of Ref. [79] extended the BKT theory, which was developed for the neutral superfluid ⁴He liquid, to thin superconducting films and showed that

$$k_{\rm B}T_{\rm BKT} = \frac{\varphi_0^2}{16\pi^2} \, \frac{1}{\Lambda(T_{\rm BKT})} \,, \tag{11}$$

where $\varphi_0 = hc/(2e)$ is the flux quantum. It turned out that in doped superconductors, $T_{\rm BKT}$ is lower than the critical Bardeen–Cooper–Schrieffer (BKS) temperature $T_{\rm c}$. We note that $T_{\rm BKT}$ does not correspond to thermodynamic instability.

It is noteworthy that we sometimes encounter a lack of understanding regarding the nature of vortices in a thin superconducting film giving rise to BKT-type transitions. These vortices are of the same nature as Abrikosov vortices in a bulk superconductor and transform into them with increasing the film thickness. The form of correction terms to Pearl's solution with the inclusion of film thickness was obtained in Ref. [81].

For T > 0, a superconducting film always has a finite free vortex density ϱ_{\pm} , with magnetic moments directed along (+)or opposite (-) the external magnetic field H. These free vortices are responsible for energy dissipation and result in the formation of a resistance 'tail' in the low-temperature region. The resistance is described by the Bardeen–Stephen formula [82]

$$\frac{R}{R_{\rm N}} = 2\pi\xi^2(\varrho_+ + \varrho_-), \qquad (12)$$

where *R* is the resistance caused by the motion of vortices, R_N is the film resistance in the normal state, and ξ is the correlation length. Consequently, the relations between the free vortex density and the temperature and field must be known for the calculation of the superconductor resistance caused by the motion of vortices. These relations can be obtained using the two-dimensional Coulomb gas theory [43] in the framework of the renormalization group method [31, 43, 83].

The existence of BKT-type transitions was confirmed experimentally in [43, 55–57, 84–88].

At the same time, there are obvious deficiencies in the description of superconducting film behavior in the framework of the two-dimensional Coulomb gas model. The form of the function $R/R_{\rm N}$ obtained using renormalization group equations can be substantiated only in a narrow temperature interval $T_{\rm BKT} < T \ll T_{\rm c}$, while the bulk of experimental results were obtained at temperatures outside this region. The renormalization group method is not applicable to superconductors at the temperatures sufficiently close to $T_{\rm BKT}$ [43]. Furthermore, the low-temperature resistance 'tail' cannot be described within the BKT theory.

Described in this section is the statistical theory of vortex plasma in two-dimensional superconductors, which overcomes some of the indicated difficulties and proposes a way of calculating the quantities in the right-hand side of Eqn (12) in the temperature range $0 < T < T_c$. The presentation is based on Refs [100–104].

2.2.1 Cycle approximation for a system of vortices in a twodimensional superconductor. We consider the free energy of a system of *N* vortices $(N = N_+ + N_-)$, whose coordinates in a sample of thickness *d* are $\mathbf{r}_i(z) = (x_i(z), y_i(z)), i = 1, ..., N$ (the external field *H* is aligned with the *z* axis). Let ε be the energy per unit vortex length. Then the free vortex energy can be represented as [82, 105-107]

$$F = \varepsilon N d + \frac{1}{2} \sum_{i \neq j}^{N} s_i s_j \int_0^d dz \, V(\mathbf{r}_i(z) - \mathbf{r}_j(z))$$

+ $\frac{1}{2} \sum_{i=1}^{N} \varepsilon \int_0^d dz \left| \frac{d\mathbf{r}_i}{dz} \right|^2,$ (13)

where $dz V(\mathbf{r}_i(z) - \mathbf{r}_j(z))$ is the interaction potential between two vortices with coordinates $\mathbf{r}_i(z)$ and $\mathbf{r}_j(z)$ in layers of thickness dz, with $s_i = \pm 1$. The last term in the right-hand side of Eqn (13) was obtained by expanding the total energy of the vortex line $E = \varepsilon \int_0^d (1 + |\mathbf{dr}_i/\mathbf{dz}|^2)^{1/2} dz$. If the vortex coordinates are assumed to vary slowly with z, it is possible to obtain the potential that is local in z: the vortices interact at the same height z. This approximation is valid for bulk samples only for vortices parallel to z. In the opposite case of a thin film, it is exactly valid in the limit $d \to 0$.

In can be shown [100–104] that the Gibbs energy of N interacting vortices is expressed as

$$G(H,T) = \left(\varepsilon - \frac{\varphi_0 H}{4\pi}\right) N_+ d + \left(\varepsilon + \frac{\varphi_0 H}{4\pi}\right) N_- d + \frac{1}{2} \sum_{i \neq j}^N s_i s_j \int_0^d dz \, V(\mathbf{r}_i(z) - \mathbf{r}_j(z)) + \frac{1}{2} \sum_{i=1}^N \varepsilon \int_0^d dz \left|\frac{d\mathbf{r}_i}{dz}\right|^2 - \frac{1}{8\pi} \frac{\mathcal{N}B^2}{1 - \mathcal{N}}, \qquad (14)$$

where *H* is the external field, *B* is the induction, and \mathcal{N} is the demagnetization coefficient. The canonical partition function for the system described by Eqn (14) is [105, 106]

$$Z_{N} = \frac{\Gamma^{N}}{N_{+}!N_{-}!} \int d\mathbf{r}_{1}' \dots \int d\mathbf{r}_{N}' \int d\mathbf{r}_{1}$$
$$\dots \int d\mathbf{r}_{N} \rho(\mathbf{r}_{1}', \dots, \mathbf{r}_{N}', \mathbf{r}_{1}, \dots, \mathbf{r}_{N}; d), \qquad (15)$$

where $(\Gamma^N/N_+!N_-!)\rho(\mathbf{r}'_1,\ldots,\mathbf{r}'_N,\mathbf{r}_1,\ldots,\mathbf{r}_N;d)$ is the partition function for N vortices with fixed endpoints: $(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ for z = 0 and $(\mathbf{r}'_1,\ldots,\mathbf{r}'_N)$ for z = d. The factor $\rho(\mathbf{r}'_1,\ldots,\mathbf{r}'_N,\mathbf{r}_1,\ldots,\mathbf{r}_N;d)$ can be represented in the form of a path integral over the vortex lines $\{\mathbf{r}_i(z)\}$:

$$\rho(\mathbf{r}'_1, \dots, \mathbf{r}'_N, \mathbf{r}_1, \dots, \mathbf{r}_N; d) = \int D\mathbf{r}_1(z) \dots \int D\mathbf{r}_N(z) \exp\left(-\beta G\right), \qquad (16)$$

where $\beta = 1/(k_BT)$ and where Feynman's definition of functional integration is used [108]. For a finite *d*, the statistical mechanics of the system described by Eqns (15) and (16) was discussed in detail in [106].

Here, we consider the opposite case $d \rightarrow 0$, which corresponds to the 'high-temperature limit' ($\beta\hbar \rightarrow 0$) for the path integral with imaginary time [108]. In this case, the Gibbs free energy G(H, T) [see Eqn (14)] in the exponent in the right-hand side of (16) can be approximated by the expression

$$G(H,T) = -\mu_{+}N_{+} - \mu_{-}N_{-} + \frac{1}{2}\sum_{i\neq j}^{N_{+}+N_{-}} s_{i}s_{j}\varPhi(r_{ij}) + \frac{1}{2}\varepsilon\sum_{i=1}^{N_{+}+N_{-}} \frac{(\mathbf{r}_{i}'-\mathbf{r}_{i})^{2}}{d} + \delta G, \qquad (17)$$

where $\mu_{+} = -[\varepsilon - \varphi_{0}H/(4\pi)]d$, $\mu_{-} = -[\varepsilon + \varphi_{0}H/(4\pi)]d$, $\Phi(r_{ij}) = dV(\mathbf{r}_{i}(0) - \mathbf{r}_{j}(0)), \ \delta G = -(8\pi)^{-1}\mathcal{N}B^{2}(1-\mathcal{N})^{-1}\Omega d$, and Ω is the area of the superconducting film.

For a thin superconducting film, the energy ε per unit vortex length has the form [80]

$$\varepsilon = \pi r_0^2 \xi^2 \left(\frac{H_c^2}{8\pi}\right) + \frac{\varphi_0^2}{16\pi\Lambda d} \left(H_0\left(\frac{\xi}{\Lambda}\right) - Y_0\left(\frac{\xi}{\Lambda}\right)\right), (18)$$

where the first term is the contribution of the vortex core, r_0 is vortex core radius (in ξ units), H_c is the thermodynamic critical field, H_0 is the Struve function, and Y_0 is the Neumann function. The interaction energy of the two vortices located at points \mathbf{r}_i and \mathbf{r}_v ($r_{ij} = |\mathbf{r}_i - \mathbf{r}_j| \ge \xi$) is [80]

$$\Phi(r_{ij}) = \frac{\varphi_0^2}{8\pi\Lambda} \left[H_0\left(\frac{r_{ij}}{\Lambda}\right) - Y_0\left(\frac{r_{ij}}{\Lambda}\right) \right],$$

$$\Phi(r_{ij}) \approx -\frac{\varphi_0^2}{4\pi^2\Lambda} \ln\frac{r_{ij}}{\Lambda}, \quad r_{ij} \ll \Lambda,$$

$$\Phi(r_{ij}) \approx \frac{\varphi_0^2}{4\pi^2 r_{ij}}, \qquad r_{ij} \gg \Lambda.$$
(19)

The corrections to this energy due to a small but finite film thickness were obtained in Ref. [81].

We substitute expression (17) in (16) and integrate over all $\{\mathbf{r}'_i\}$ in the sum in (15) to find

$$Z_N = \exp\left(-\beta\delta G\right) \frac{z_+^{N_+} z_-^{N_-}}{N_+! N_-!} \\ \times \int d\mathbf{r}_1 \dots \int d\mathbf{r}_N \exp\left(-\frac{\beta}{2} \sum_{i \neq j} s_i s_j \Phi(r_{ij})\right), \qquad (20)$$

where the activities z_{\pm} and z_{-} are of the form $z_{\pm} = \Gamma \exp(\beta \mu_{\pm})$.

We estimate the constant Γ . Setting N = 1 and H = 0 in Eqn (20), we obtain $(z_+ = z_- = z)$

$$Z_1 = z\Omega. (21)$$

The vortex free energy corresponding to the partition function Z_1 must be equal to the energy of creating a single vortex oriented perpendicular to the film (in the limit $L \rightarrow \infty$):

$$F_{\rm vor} = \varepsilon d - TS \,. \tag{22}$$

The entropy *S* has the form $S = \ln (\Omega/\zeta)$, where ζ is the area occupied by the vortex. It is assumed that ζ is proportional to the area of the domain occupied by the vortex core: $\zeta = c\xi^2$, where *c* is a temperature-independent constant [43]. We use formulas (21) and (22) to obtain

$$\Gamma = \frac{1}{c\xi^2} \,. \tag{23}$$

The grand canonical partition function is of the form

$$Z = \exp\left(-\beta\delta G\right) \sum_{N_+,N_-=0}^{\infty} \frac{z_+^{N_+} z_-^{N_-}}{N_+! N_-!} \int d\mathbf{r}_1 \dots \int d\mathbf{r}_N$$
$$\times \exp\left(-\frac{\beta}{2} \sum_{i \neq j} s_i s_j \Phi(r_{ij})\right) = \exp\left(-\beta\delta G\right) Z'.$$
(24)

The sum in (24) is taken over all configurations with different N_+ and N_- .

The Gibbs free energy associated with (24) is expressed as [73]

$$G = -k_{\rm B}T \ln Z = \delta G + k_{\rm B}T \left[\varrho_+ \left(\ln \frac{\varrho_+}{z_+} - 1 \right) + \varrho_- \left(\ln \frac{\varrho_-}{z_-} - 1 \right) - S \right] \Omega, \quad (25)$$

$$S = \sum_{n_{+}+n_{-} \ge 2} \sum_{n_{+}} \sum_{n_{-}} \beta_{n_{+}n_{-}} \varrho_{+}^{n_{+}} \varrho_{-}^{n_{-}} , \qquad (26)$$

where β_{n+n} is the sum of irreducible Mayer diagrams [73],

$$\beta_{n_{+}n_{-}} = (n_{+}!n_{-}!\Omega)^{-1} \int d\mathbf{r}_{1} \dots d\mathbf{r}_{\nu} \sum \prod f_{ij},$$

$$f_{ij} = \exp\left(-\beta \Phi(r_{ij})\right) - 1.$$
(27)

Here, $v = n_+ + n_-$, the product operator corresponds to connected diagrams without nodal vertices, for which 1 < i < j < v, and the sum is taken over all such diagrams.

The induction *B* is related to the free vortex densities ρ_+ and ρ_- as $B = \varphi_0(\rho_+ - \rho_-)$. Substituting this formula in expression (25) gives *G* as a function of *T*, *H*, ρ_+ , and ρ_- .

To obtain the equations for ρ_+ and ρ_- , we use the virial expansion [73, 109]

$$\varrho_{\pm} = z_{\pm} \exp\left(\frac{\partial}{\partial \varrho_{\pm}} S\right). \tag{28}$$

We note that Eqn (28) can be derived from the extremum condition for the free energy G:

$$\frac{\partial G}{\partial \varrho_+} = \frac{\partial G}{\partial \varrho_-} = 0.$$
⁽²⁹⁾

The long-range nature of interaction (19) gives rise to the problem of convergence of certain terms in Mayer expansion (26). This problem can be solved using the cycle approximation, which is well known in plasma physics. In this approximation [109],

$$S = \sum_{\nu \ge 2} S_{\nu},$$

$$S_{\nu} = \sum_{n_{+}} \sum_{n_{-}} \frac{(\nu - 1)!}{2} \frac{(-\beta \varrho_{+})^{n_{+}}}{n_{+}!} \frac{(-\beta \varrho_{-})^{n_{-}}}{n_{-}!} J_{\nu}$$

$$= \frac{1}{2\nu} \left[-\beta(\varrho_{+} + \varrho_{-}) \right]^{\nu} J_{\nu},$$
(30)

where $J_{\nu} = \Omega^{-1} \int d\mathbf{r}_1 \dots d\mathbf{r}_{\nu} \Phi(r_{12}) \Phi(r_{23}) \dots \Phi(r_{\nu 1})$. The quantity J_{ν} can be calculated using the Fourier transformation and taking into account that the Fourier transform $\tilde{\Phi}(q)$ of potential (19) has the form

$$\tilde{\Phi}(q) = \frac{\varphi_0^2}{2\pi\Lambda} \frac{1}{q(q+1/\Lambda)} \,. \tag{31}$$

Calculations with Eqns (30) and (31) show that

$$= \begin{cases} \frac{1}{2} \kappa^{2} - \frac{1}{2} \left(\kappa^{2} - \frac{1}{2\Lambda^{2}} \right) \ln \left(\kappa^{2} \Lambda^{2} \right) - \frac{\omega}{\Lambda} \arctan \left(2\omega\Lambda \right), \\ \kappa^{2} - \frac{1}{4\Lambda^{2}} \ge 0, \\ \frac{1}{2} \kappa^{2} - \frac{1}{2} \left(\kappa^{2} - \frac{1}{2\Lambda^{2}} \right) \ln \left(\kappa^{2}\Lambda^{2} \right) + \frac{\sigma}{2\Lambda} \ln \frac{1 + 2\Lambda\sigma}{1 - 2\Lambda\sigma}, \\ \kappa^{2} - \frac{1}{4\Lambda^{2}} < 0, \end{cases}$$
(32)

where $\kappa^2 = \beta(\varrho_+ + \varrho_-) \varphi_0^2 / (2\pi\Lambda)$, $\omega = (\kappa^2 - 1/(4\Lambda^2)^{1/2})$, and $\sigma = (1/(4\Lambda^2) - \kappa^2)^{1/2}$.

2.2.2 Vortex system in the absence of a magnetic field. We discuss the properties of a superconducting magnetic film in the absence of an external magnetic field. In this case, $\rho_+ = \rho_- = \rho/2$ and $z_+ = z_- = z$. Substitution of formulas (32) in expression (28) gives

$$\varrho = 2z \exp\left[\beta \frac{\varphi_0^2}{16\pi^2 \Lambda} \left(\ln\left(\kappa^2 \Lambda^2\right) + \frac{1}{\omega \Lambda} \arctan\left(2\omega\Lambda\right)\right)\right],$$

$$\kappa^2 - \frac{1}{4\Lambda^2} \ge 0, \qquad (33)$$

$$\begin{split} \varrho &= 2z \exp\left[\beta \frac{\varphi_0^2}{16\pi^2 \Lambda} \left(\ln\left(\kappa^2 \Lambda^2\right) + \frac{1}{2\sigma\Lambda} \ln\frac{1+2\sigma\Lambda}{1-2\sigma\Lambda}\right)\right],\\ &\kappa^2 - \frac{1}{4\Lambda^2} < 0\,, \end{split} \tag{34}$$

where $\kappa^2 = \beta \varrho \varphi_0^2 / (2\pi \Lambda)$.

 $\alpha(\mathbf{m})$

Using Eqns (25) and (32), we write G(T) as

$$\begin{aligned} \frac{G(T)}{k_{\rm B}T\Omega} &= \rho \left(\ln \frac{\rho}{2z} - 1 \right) + \frac{1}{4\pi} \\ \times \begin{cases} \frac{1}{2} \kappa^2 - \frac{1}{2} \left(\kappa^2 - \frac{1}{2\Lambda^2} \right) \ln \left(\kappa^2 \Lambda^2 \right) - \frac{\omega}{\Lambda} \arctan \left(2\omega\Lambda \right), \\ \kappa^2 - \frac{1}{4\Lambda^2} &\ge 0, \end{aligned} \right. \tag{35} \\ \frac{1}{2} \kappa^2 - \frac{1}{2} \left(\kappa^2 - \frac{1}{2\Lambda^2} \right) \ln \left(\kappa^2 \Lambda^2 \right) + \frac{\sigma}{2\Lambda} \ln \frac{1 + 2\Lambda\sigma}{1 - 2\Lambda\sigma}, \\ \kappa^2 - \frac{1}{4\Lambda^2} &< 0. \end{aligned}$$

By substituting Eqns (33) and (34) in formulas (35), we express the free energy in the form of the 'equation of state' [73, 109]:

$$\frac{P}{k_{\rm B}T} = \varrho - 2\varrho \frac{\partial S}{\partial \varrho} + S \,,$$

where the vortex plasma pressure is $P = -G(T)/\Omega$.

The behavior of ρ as a function of *T* in the vicinity of T_{BKT} and for low *T* can be obtained in explicit form. We consider these cases.

For $T \rightarrow 0$, as is seen from Eqn (34), the vortex density $\rho \rightarrow 0$,

$$\varrho = \frac{2}{c\xi^2} \exp\left(-\frac{\varepsilon d}{k_{\rm B}T}\right). \tag{36}$$

We now consider approximate solutions of Eqns (33) and (34) in the vicinity of T_{BKT} . In this case, Eqn (33) has to be solved, because the inequality $\kappa^2 - 1/(4\Lambda^2) \ge 0$ is satisfied for a nonzero ϱ and a sufficiently small thickness *d*. In the small-*d* limit, the second term in the exponent in Eqn (33) can be disregarded and Eqn (33) reduces to

$$\kappa^2 \Lambda^2 = \frac{z\beta\varphi_0^2 \Lambda}{\pi} \exp\left[\beta \frac{\varphi_0^2}{16\pi^2 \Lambda} \ln\left(\kappa^2 \Lambda^2\right)\right].$$
 (37)

The solution of Eqn (37) is of the form

$$\varrho = \frac{2\pi k_{\rm B}T}{\varphi_0^2 \Lambda} q^{k_{\rm B}T/(k_{\rm B}T - \Theta(T))}, \qquad (38)$$

where $q = z\beta\varphi_0^2 \Lambda/\pi$ and $\Theta(T) = \varphi_0^2/(16\pi^2\Lambda(T))$. Equation (38) is similar to the equation used to describe the Kosterlitz– Thouless transition [43]. In accordance with Eqn (38), $\rho \to 0$ as $T \to T_{BKT}$ from above, where T_{BKT} is defined by the equation $k_B T_{KT} = \Theta(T_{BKT})$ [see Eqn (11)] (when q < 1).

Incidentally, for exact equations (33) and (34), there is no phase transition in the sense that the vortex density ρ never vanishes exactly, but ρ varies quite rapidly in the vicinity of T_{BKT} due to the dissociation of vortex–antivortex pairs.

Parameters for specific calculations were borrowed from experimental paper [85], where the properties of a 20 Å thick Nb film were studied in detail. In this case,

$$\xi(t) = \xi(0)/\sqrt{1-t}$$
 and $\lambda_{\rm B}(t) = \lambda(0)/\sqrt{1-t}$,

where $t = T/T_c$, $T_c \simeq 3.66$ K, $\xi(0) \simeq 104$ Å, and $\lambda(0) \simeq 1600$ Å; T_c is defined as the temperature at which $R = 0.5R_N$. The constant *c* can be determined from this condition. Using formulas (12), (23), and (33), we obtain $c = 6\pi$. The derivation of the core radius r_0 is described in detail in what follows. The calculations were done for two r_0 values: 1.25 and 2.3. (The latter estimate was borrowed from Ref. [53].) In general, r_0 can be considered a tunable parameter.

2.2.3 Dependence of the phase transition on the vortex core radius (or vortex core energy). As discussed above, the form of the solutions of Eqns (33) and (34) depends on the vortex core radius r_0 because of relation (18) between r_0 and the vortex core energy.

We represent Eqn (33) in the form [see Eqn (38)]

$$\varrho = \frac{2\pi k_{\rm B}T}{\varphi_0^2 \Lambda} q^{k_{\rm B}T/(k_{\rm B}T - \Theta(T))} \\
\times \exp\left[\frac{\Theta(T)}{k_{\rm B}T - \Theta(T)} \frac{1}{\omega\Lambda} \arctan\left(2\omega\Lambda\right)\right].$$
(39)

It follows from Eqn (39) that for q < 1, the free vortex density $\rho \to \infty$ as *T* tends to T_{BKT} from below. On the other hand, for q > 1, the density ρ tends to infinity as *T* approaches T_{BKT} from above. The critical value of the vortex core radius r_0^c can be found from the equation $q(T_{BKT}, r_0) = 1$, whence $r_0^c = 1.2237$.

The behavior of the solutions of Eqns (33) and (34) (see Refs [100–102]) can be regarded as an indication that the dissociation of vortex pairs for $r_0 < r_0^c$ occurs via a first-order transition. However, we note the obvious drawbacks of these solutions. First, the free vortex density tends to infinity as $T_{\rm BKT}$ is approached from above. Furthermore, there is a small neighborhood of $T_{\rm BKT}$ in which the solution is not defined. The possible reason why the free-vortex density tends to infinity can be the fact that Eqns (33)–(35) were derived with the use of the point-like vortex assumption, whereby the core radius appears in the equations only via the vortex core energy.

To take the finite size of the vortex core into account, we represent the interaction energy in the form [43, 52]

$$\tilde{\boldsymbol{\Phi}}(r) = \int \mathrm{d}^2 r' \, \mathrm{d}^2 r'' \, n\big(|\mathbf{r} - \mathbf{r}'|\big) \, \boldsymbol{\Phi}\big(|\mathbf{r}' - \mathbf{r}''|\big) \, n(r'') \,, \qquad (40)$$

where n(r) is the 'charge' distribution of a single vortex, $\int n(r) d^2r = 1.$

The Fourier transform of the potential $\tilde{\Phi}(r)$ has the form

$$\tilde{\varPhi}_q = \frac{\varphi_0^2}{2\pi\Lambda} \frac{n_q^2}{q(q+1/\Lambda)} , \qquad (41)$$

where n_q is the Fourier transform of the charge distribution n(r) of a single vortex,

$$n_q = \int d^2 r \, \exp\left(i\mathbf{q}\mathbf{r}\right) n(r) \,, \tag{42}$$

n(r) = 0 for $r \to \infty$, and $n(r) \neq 0$ in the neighborhood $r \leq \xi$.

Using the cycle approximation, it is easy to show that the free energy G for non-point-like vortices with interaction (40) is expressed as

$$\frac{G}{k_{\rm B}T\Omega} = 2\varrho \left(\ln \frac{\varrho}{2z} - 1 \right) + \frac{1}{8\pi^2} \int d^2q \left[\ln(1 + \kappa^2 \tilde{u}_q) - \kappa^2 \tilde{u}_q \right],$$
(43)

where

$$\tilde{u}_q = \frac{n_q^2}{q(q+1/\Lambda)} \,. \tag{44}$$

To obtain the equations for ρ , we use the virial expansion [73] or the extremum condition for the energy *G*,

$$\frac{\partial G}{\partial \varrho} = 0. \tag{45}$$

From Eqns (43) and (45), we have

$$\ln \frac{\varrho}{2z} = -\frac{1}{8\pi^2} \frac{\partial}{\partial \varrho} \int d^2 q \left[\ln \left(1 + \kappa^2 \tilde{u}_q \right) - \kappa^2 \tilde{u}_q \right].$$
(46)

We choose the following n(r) distribution:

$$n(r) = \int_{q \leq B} \frac{\mathrm{d}^2 q}{4\pi^2} \exp\left(-\mathrm{i}\mathbf{q}\mathbf{r}\right). \tag{47}$$

From Eqn (47), we obtain

$$n_q = \begin{cases} 1, & q \leq B, \\ 0, & q > B. \end{cases}$$

$$\tag{48}$$

We note that the behavior of the two-dimensional Coulomb gas depends only weakly on the specific form of the charge distribution [53, 54, 70, 71]. In much the same way, it can be assumed that simple equations (47) and (48) are sufficient to describe the vortex–antivortex pair dissociation in a two-dimensional superconductor. To determine the parameter B, we note that two vortices with opposite signs placed at the same point must annihilate. The energy of two opposite vortices that are perpendicular to the superconductor plane and are located at a distance r from each other can be represented in the form

$$\Delta F_{\text{pair}}(r) = 2\varepsilon + \tilde{\Phi}(r) \,, \tag{49}$$

where the energy of a single vortex is [see Eqn (18)]

$$\varepsilon = \pi r_0^2 \xi^2 d \, \frac{H_c^2}{8\pi} + \frac{\varphi_0^2}{16\pi \Lambda} \left(H_0\left(\frac{\xi}{\Lambda}\right) - Y_0\left(\frac{\xi}{\Lambda}\right) \right). \tag{50}$$

Using the condition $\Delta F_{\text{pair}}(0) = 0$, we obtain the equation for *B*. It can be shown that $B \simeq 1/\xi$ for $\xi \ll \Lambda$, i.e., in the limit $\xi \to 0$ we have $n(r) \to \delta(r)$. We use Eqns (46) and (48) to find

$$\ln\frac{\varrho}{2z} = \frac{\beta\varphi_0^2}{16\pi^2\Lambda} \left\{ \ln\left[\frac{(B+1)^2}{B^2 + B + \zeta}\zeta\right] + J(B,\zeta) \right\},\tag{51}$$

where

$$J(B,\zeta) = \begin{cases} \frac{2}{\sqrt{4\zeta - 1}} \left(\arctan \frac{2B + 1}{\sqrt{4\zeta - 1}} - \arctan \frac{1}{\sqrt{4\zeta - 1}} \right), & 4\zeta - 1 \ge 0, \\ \frac{1}{\sqrt{1 - 4\zeta}} \ln \left(\frac{2B + 1 - \sqrt{1 - 4\zeta}}{2B + 1 + \sqrt{1 - 4\zeta}} \right) \frac{1 + \sqrt{1 - 4\zeta}}{1 - \sqrt{1 - 4\zeta}}, & 4\zeta - 1 \le 0, \end{cases}$$
(52)

and $\zeta = \kappa^2 \Lambda^2$. For $B \to \infty$, Eqn (51) reduces to the point-like limit in Eqns (33) and (34).

Figure 4 shows the behavior of $\log_{10}(R/R_N)$ with temperature. The values of $\log_{10}(R/R_N)$ were calculated from Eqn (51) with $r_0 = 1.25$. The dotted curve shows the solution of Eqn (51) corresponding to the limit $B \to \infty$. We can see that the transition becomes broader, but the behavior remains qualitatively the same. As discussed above, the behavior of the solution changes qualitatively for r_0 smaller than the critical value $r_0^c = 1.22$. Figure 5 shows the solution of Eqn (51) for $r_0 = 0.9$, corresponding to the non-point-like limit in (40). The dotted line that runs to the left in Fig. 5 shows the nonphysical solution corresponding to the 'pointlike' limit $B \to \infty$.



Figure 4. Temperature dependence of $\log_{10}(R/R_N)$ calculated by Eqn (51) with $r_0 = 1.25$.



Figure 5. Temperature dependence of $\log_{10}(R/R_N)$ calculated by Eqn (51) with $r_0 = 0.9$.



Figure 6. Temperature dependence of the Gibbs free energy $G(T)/(k_B\Omega)$ corresponding to the solid curve in Fig. 5.

The S-like structure of the $\log_{10} (R/R_N)$ curve is characteristic of a first-order transition. The transition temperature can be calculated from the plot in Fig. 6, which shows the Gibbs free energy $G(T)/(k_B\Omega)$ corresponding to the solid curve in Fig. 5. The transition temperature is $T_1 = 3.6396$ K, $T_1 < T_{BKT}$ (the vertical line in Fig. 5).

Thus, our treatment is based on the explicit equations for the free vortex density and Gibbs free energy derived within the cycle approximation in the case of long-range intervortex potential (19). In the absence of an external magnetic field for high core energies, the free vortex density ρ is nonzero for arbitrary $T \neq 0$, but one can speak about the BKT transition in the sense that ρ varies quite rapidly in the vicinity of T_{BKT} . For low core energies, the vortex– antivortex pair dissociation occurs by means of a first-order transition, the transition temperature depending on the core energy.

The cycle approximation was developed for studying the three-dimensional plasma properties [73, 109]. It was natural to attempt to use this approximation in the two-dimensional case. In two dimensions, there are two kinds of long-range potentials that are commonly considered: the logarithmic potential, which is a solution of the two-dimensional Poisson equation and is referred to as the two-dimensional Coulomb potential (two-dimensional Coulomb gas [43]), and the ordinary three-dimensional Coulomb potential of the form 1/r used, for instance, to describe a two-dimensional electron system.

It can be shown that the application of the cycle approximation to these potentials gives rise to the respective infrared and ultraviolet divergences of thermodynamic functions. Formula (19) for the intervortex interaction potential can be considered an interpolating relation between the formulas describing these two potentials, with the result that the theory outlined above is free of divergences in the absence of a magnetic field.

The experimentally observed transition (see, e.g., Fig. 9 in Ref. [85]) is in good qualitative agreement with the data given in Fig. 4, but is broader. This discrepancy, in our view, is attributable to the fact that the proposed theory neglects pinning, which is always present in experimental samples. The influence of pinning results in additional dissociation of vortex–antivortex pairs (see, e.g., Ref. [99]), which in turn must entail an additional broadening of the curves plotted in Fig. 4.

3. Two-dimensional melting

3.1 Special features of crystal ordering in two dimensions

The nature of two-dimensional melting has been the subject of intense discussion over the last 40 years [110-114]. Considerable progress in explaining two-dimensional melting was made after the advent of the theory by Halperin and Nelson [37, 38] and Young [39] based on the ideas of Berezinskii, Kosterlitz, and Thouless (the BKTHNY theory). This theory predicts that melting in the two-dimensional case can be fundamentally different from the melting of ordinary three-dimensional systems [32, 115]. In comparison to an isotropic liquid, two symmetries are violated in a three-dimensional solid crystal: translational and rotational. These symmetries are not independent. Indeed, rotation of one part of an ideal crystal relative to another breaks not only orientational correlations but also translational ones. However, we can imagine a state of a condensed medium with long-range correlations between the directions of local crystallographic axes but without a long-range translational order [116–121]. The notion of anisotropic liquids of this kind is an important part of modern melting theories of twodimensional systems.

Due to well-developed fluctuations, the properties of twodimensional crystals are significantly different from the properties of three-dimensional ones. Even in the mid-1930s, Peierls and Landau [122–124] independently adduced arguments that a periodic lattice cannot exist in the cases of one and two dimensions. Peierls's arguments were based on the harmonic approximation in the crystal theory. Landau used his theory of phase transitions [14].

We briefly consider the properties of crystal ordering in two dimensions [125, 126]. The two-dimensional analogue of an ordinary three-dimensional crystal can be described by a local density of the form $\rho(x, y) = \sum_{\mathbf{R}} \rho_{\mathbf{A}}(\mathbf{r} - \mathbf{R})$, where $\rho_{\mathbf{A}}(\mathbf{r})$ is the density function of a single atom and {**R**} is a two-dimensional lattice site. We let $\mathbf{u}(x, y)$ denote the displacement vector of some small crystal domain, the displacement being due to thermodynamic fluctuations at $T \neq 0$. The probability of a fluctuation w characterized by a vector \mathbf{u} is $w \propto \exp[-\delta F/(k_{\mathbf{B}}T)]$, where $\delta F = \int (F - \overline{F}) d^2 r$ is the deviation of the total energy of the system from the mean value \overline{F} , and F is the free energy per unit area of the twodimensional system. The mean value of a quantity $\langle A \rangle$ is calculated as [125]

$$\langle A \rangle = \frac{\sum_{\mathbf{u}(\mathbf{r})} A \exp\left[-\delta F/(k_{\rm B}T)\right]}{\sum_{\mathbf{u}(\mathbf{r})} \exp\left[-\delta F/(k_{\rm B}T)\right]} ,$$

with the summation performed over all possible vectors $\{\mathbf{u}\}$.

In the harmonic approximation, the free-energy functional is of the form

$$\delta F[\mathbf{u}(\mathbf{r})] = \frac{1}{2} \int \lambda_{ijlm} \frac{\partial u_i}{\partial x_j} \frac{\partial u_l}{\partial u_m} d^2 r,$$

where λ_{ijlm} is the tensor of elastic moduli [127]. The vector $\mathbf{u}(\mathbf{r})$ can be expanded in a Fourier series

$$\mathbf{u}(\mathbf{r}) = \sum_{\mathbf{k}} \mathbf{u}_{\mathbf{k}} \exp\left(\mathbf{i}\mathbf{k}\mathbf{r}\right),$$

where $\mathbf{u}_{-\mathbf{k}} = \mathbf{u}_{\mathbf{k}}^*$, $k \leq 1/d$, and *d* is the linear size of the domain characterized by the vector $\mathbf{u}(\mathbf{r})$. In this case, δF takes the form

$$\delta F[\mathbf{u}] = \frac{1}{2} V \sum_{\mathbf{k}} \lambda_{ijlm} k_j k_m u_{i\mathbf{k}} u_{l\mathbf{k}}^* = \frac{1}{2} V \sum_{\mathbf{k}} \beta_{il}(\mathbf{k}) u_{i\mathbf{k}} u_{l\mathbf{k}}^*,$$

where *V* is the volume of the system and the elements of the real tensor $\beta_{il}(\mathbf{k})$ are quadratic functions of the components of the **k** vector. By the quadraticity of the expression for δF , the mean-square fluctuations of $\mathbf{u}_{\mathbf{k}}$ have the form

$$\langle u_{i\mathbf{k}}u_{l\mathbf{k}}^{*}\rangle = \frac{k_{\mathrm{B}}T}{V}\beta_{il}^{-1}(\mathbf{k}),$$

where β_{ik}^{-1} is the inverse tensor to β_{il} . The tensor $\beta_{il}^{-1}(k)$ can be written in the form $[A_{il}(\hat{\mathbf{n}})]k^2$, where A_{il} depends only on the direction of $\mathbf{k} : \hat{\mathbf{n}} = \mathbf{k}/k$.

The mean-square displacement $\langle |\mathbf{u}|^2 \rangle$ is found by summing over **k**. We replace the sum over **k** with integration to obtain

$$\langle |\mathbf{u}|^2 \rangle = k_{\rm B} T \int \frac{A_{ii}(\hat{\mathbf{n}})}{k^2} \frac{\mathrm{d}^2 k}{(2\pi)^2} = \frac{k_{\rm B} T}{(2\pi)^2} \int_0^{2\pi} A_{ii}(\varphi) \,\mathrm{d}\varphi \, \int_0^{1/d} \frac{\mathrm{d}k}{k} \,.$$
 (53)

The integral over k diverges logarithmically as $k \to 0$, which has the result that the fluctuation displacement tends to infinity logarithmically in the thermodynamic limit of an infinite system. Therefore, a two-dimensional harmonic crystal is devoid of two-dimensional translational order: this order is destroyed by thermodynamic fluctuations at a finite temperature.

Nonetheless, it is noteworthy that the logarithmic divergence is very slow (for instance, according to the estimates in [128], a fluctuation displacement of the order of 10 interatomic distances emerges in a system in which the number of particles exceeds the number of atoms in the observable Universe). Therefore, experimental systems can be treated as two-dimensional crystals with a rather high degree of accuracy.

Expression (53) defines the mean-square fluctuation displacement at each point of a two-dimensional crystal. A more rigorous explanation of the behavior of such systems can be achieved by considering fluctuation correlations at different points of the system [125].

At T = 0, a two-dimensional lattice exists irrespective of its size, because the divergence arises primarily from thermal fluctuations. Let $\rho_0(\mathbf{r})$ be the density function of the system at T = 0. At sufficiently low temperatures, only long-wavelength fluctuations exist in the system, i.e., $\mathbf{u}(\mathbf{r})$ changes little over a distance of the order of the lattice constant *a* (which corresponds to short-wave-vector fluctuations). In this case, the density can be represented in the form $\rho(\mathbf{r}) = \rho_0(\mathbf{r} - \mathbf{u}(\mathbf{r}))$ and the fluctuation correlation is defined by the expression

$$\left\langle \rho(\mathbf{r}_1) \, \rho(\mathbf{r}_2) \right\rangle = \left\langle \rho_0 \big[\mathbf{r}_1 - \mathbf{u}(\mathbf{r}_1) \big] \, \rho_0 \big[\mathbf{r}_2 - \mathbf{u}(\mathbf{r}_2) \big] \right\rangle. \tag{54}$$

The function $\rho_0(\mathbf{r})$ can be expanded in the Fourier series in reciprocal lattice vectors:

$$\rho_0(\mathbf{r}) = \bar{\rho} + \sum_{\mathbf{G} \neq 0} \rho_{\mathbf{G}} \exp\left(\mathrm{i}\mathbf{G}\mathbf{r}\right)$$

We substitute this expression in expression (54) and use the average of the form

$$\langle \exp\left[-\mathrm{i}\mathbf{G}(\mathbf{u}_{1}-\mathbf{u}_{2})\right] \rangle = \exp\left(-\frac{1}{2} G_{i}G_{l}\chi_{il}\right),$$

$$\chi_{il}(\mathbf{r}) = \langle (u_{i1}-u_{i2})(u_{l1}-u_{l2}) \rangle$$

$$= k_{\mathrm{B}}T \int \frac{A_{il}(\hat{\mathbf{n}})}{k^{2}} 2\left[1-\cos\left(\mathbf{kr}\right)\right] \frac{\mathrm{d}k_{x}\,\mathrm{d}k_{y}}{(2\pi)^{2}}$$

$$\approx \frac{k_{\mathrm{B}}T}{\pi} \bar{A}_{il}\ln\left(k_{\mathrm{max}}r\right),$$

to obtain

ſ

$$g_{\mathbf{G}}(|\mathbf{r}_{1}-\mathbf{r}_{2}|) = \left\langle \rho(\mathbf{r}_{1}) \, \rho(\mathbf{r}_{2}) \right\rangle - \bar{\rho}^{2} \propto \frac{1}{r^{k_{\mathrm{B}}T\alpha_{G}}} \cos\left(\mathbf{G}\mathbf{r}\right),$$

$$\alpha_{G} = \frac{G_{i}G_{l}\bar{A_{il}}}{2\pi},$$
(55)

where **G** is taken as the principal period of the reciprocal lattice with the smallest α_G , and \overline{A}_{il} is the average over the inplane directions of **k**.

Although correlations decaying in accordance with a power law formally rule out long-range order, a twodimensional harmonic crystal nevertheless has a high degree of ordering. The structure factor of the two-dimensional crystal has the form

$$S(q) = \beta \int d\mathbf{r} \exp(-i\mathbf{q}\mathbf{r}) \left\langle \rho(0) \rho(\mathbf{r}) \right\rangle$$

= $\beta \int d\mathbf{r} \exp(-i\mathbf{q}\mathbf{r}) \frac{\exp(i\mathbf{G}\mathbf{r})}{r^{\eta_G}}$
= $\frac{\beta}{|\mathbf{G}-\mathbf{q}|^{2-\eta_G}} \int_0^\infty x^{1-\eta_G} dx \int_0^{2\pi} d\phi \exp(-ix\cos\phi).$ (56)

The remaining integral is model-independent and is a constant, with the temperature dependence absorbed into in the first factor. Therefore, the power-law singularity replaces the δ -like one typical of a three-dimensional crystal. In real experiments, it is sometimes rather difficult to distinguish a power-law correlation function decay from a true long-range order. The ordering with a slow power-law decaying correlation is commonly referred to as a quasi-long-range order. It is a consequence of the dimensionality of the system.

But there is a true long-range order in two-dimensional systems, the bond orientation order. In 1968, Mermin [36] considered the behavior of crystal ordering in a two-dimensional system of particles interacting via a pair potential. Assuming rather general boundary conditions, he showed that the Fourier components of the density with $k \neq 0$ vanish in the thermodynamic limit, i.e., the system has no periodic long-range order. Mermin also showed that the averaged direction of the vector connecting any two neighboring atoms at a finite temperature is the same as the direction of this vector at T = 0, i.e., the two-dimensional lattice has a long-range order.

To illustrate the behavior of orientational ordering, we consider a harmonic crystal. In the continuous approximation, the angle between the local crystallographic axis and some axis of the ideal lattice has the form

$$\vartheta(x,y) = \frac{1}{2} \left(\partial_x u_y - \partial_y u_x \right).$$
(57)

Using the Fourier expansion of $\vartheta(x, y)$,

$$\vartheta(x, y) = \frac{1}{2} \sum_{\mathbf{k}} (ik_x u_{y,\mathbf{k}} - ik_y u_{x,\mathbf{k}}) \exp(i\mathbf{k}\mathbf{r}), \qquad (58)$$

for the mean $\langle \vartheta^2 \rangle$ we obtain the expression

$$\langle \vartheta^2 \rangle = \frac{k_{\rm B}T}{(4\pi)^2} \sum_{ij} \int_0^{2\pi} f_i(\varphi) f_j(\varphi) A_{ij}(\hat{n}) \,\mathrm{d}\varphi \int_0^{1/d} k \,\mathrm{d}k \,,$$

where $f_x(\varphi) = \cos \varphi$ and $f_y(\varphi) = \sin \varphi$. Therefore, the mean square of the fluctuations of the angle $\vartheta(x, y)$ remains finite even for an infinite sample, i.e., the orientation of the bond direction 'propagates' throughout the crystal.

The correlation function of bond directions has the form

$$\left\langle \vartheta(\mathbf{r}_1) \,\vartheta(\mathbf{r}_2) \right\rangle = \frac{k_{\rm B}T}{(4\pi)^2} \sum_{ij} \int_0^{2\pi} f_i(\varphi) \,f_j(\varphi) \\ \times A_{ij}(\hat{\mathbf{n}}) \,\mathrm{d}\varphi \int_0^{1/d} \cos\left[\mathbf{k}(\mathbf{r}_1 - \mathbf{r}_2)\right] k \,\mathrm{d}k$$

This expression is finite even for $r \to \infty$, and hence the orientational order is a long-range one.

Prior to considering modern theories of two-dimensional melting, we emphasize that owing to the high ordering of a two-dimensional lattice, topological defects like dislocations and disclinations turn out to be well defined despite the absence of the long-range periodic translational order. This is significant because it is precisely dislocations and disclinations that play the main role in modern theories of twodimensional melting.

3.2 Berezinskii–Kosterlitz–Thouless–Halperin–Nelson– Young theory

As discussed in Section 3.1, the BKTHNY theory, based on considering the behavior of topological defects—dislocations and disclinations—predicts that melting can occur by means of two continuous transitions. At the same time, there are several theories predicting that the melting can occur by a first-order transition. This contradiction has spawned a large number of experimental studies and computer simulations, but this issue has not been completely clarified.

In the BKTHNY theory, two-dimensional melting was treated in the framework of the BKT theory, but with some complications imposed by the specific symmetry of the crystal lattice. As mentioned in Section 2, the crystal lattice is characterized by two kinds of broken symmetry: translational and rotational, which correspond to two different order parameters and, accordingly, two types of topological defects: dislocations (Fig. 7) and disclinations (Fig. 8). Below, we outline the main results of the BKTHNY theory.

The BKTHNY theory is based on considering the elastic Hamiltonian for a two-dimensional triangular lattice [127]

$$H_E = \frac{1}{2} \int d^2 r \left(2\mu u_{ij}^2 + \lambda u_{kk}^2 \right),$$
 (59)

where

$$u_{ij} = \frac{1}{2} \left(\frac{\partial u_i(\mathbf{r})}{\partial r_j} + \frac{\partial u_j(\mathbf{r})}{\partial r_i} \right)$$
(60)

and μ and λ are Lamé coefficients.



Figure 7. Dislocation as a disclination dipole.



Figure 8. (a) Positive, s = +1, and (b) negative, s = -1, disclinations.

The quasi-long-range periodic translational order is destroyed due to the production of free dislocations (which play the role of vortices in the XY model). The appearance of free dislocations has the result that the shear modulus μ vanishes. The main difference of the dislocation melting theory from the vortex-antivortex pair dissociation in the XY model, which was discussed in Section 2, is that a dislocation is described by the Burgers vector **b** rather than a scalar charge [see formula (6)]. The dislocation at a point **r** is defined by the increment acquired by the contour integral of the displacement field taken over a closed contour around the dislocation [127] (see Fig. 7):

$$\oint \mathbf{d}\mathbf{u} = a_0 \mathbf{b}(\mathbf{r}) = -n(\mathbf{r}) a_0 \mathbf{e}_1 - m(\mathbf{r}) a_0 \mathbf{e}_2 , \qquad (61)$$

where $\mathbf{b}(\mathbf{r})$ is the dimensionless Burgers vector, a_0 is the spacing of the triangular lattice under consideration, \mathbf{e}_1 and \mathbf{e}_2 are the basis vectors of the lattice, and *m* and *n* are integers.

A disclination in a triangular lattice has the property that the integral of rotation angle (57) taken along a closed contour enclosing the disclination acquires an increment that is a multiple of $2\pi/6$ (see Fig. 8):

$$\oint \mathbf{d}\vartheta(\mathbf{r}) = -\frac{2\pi}{6}\,s\,,\qquad s = \pm 1, \pm 2, \dots\,. \tag{62}$$

(The contours in integrals (61) and (62) run in the counterclockwise direction.) As is evident from Fig. 7, a dislocation can be considered as a coupled pair of disclinations.

The energy of a single dislocation diverges logarithmically with the size of the system. The Hamiltonian of the system of dislocations is [37, 39]

$$H_{\text{dis}} = -\frac{a_0^2 K}{8\pi} \sum_{i \neq j}^{M} \left[\mathbf{b}(\mathbf{r}_i) \, \mathbf{b}(\mathbf{r}_j) \ln \frac{r_{ij}}{a} - \frac{(\mathbf{b}(\mathbf{r}_i) \, \mathbf{r}_{ij})(\mathbf{b}(\mathbf{r}_j) \, \mathbf{r}_{ij})}{r_{ij}^2} \right] + E_{\text{c}} \sum_{i=1}^{M} \mathbf{b}^2(\mathbf{r}_i) \,, \tag{63}$$

where E_c is the dislocation core energy and K is the Young modulus,

$$K = \frac{4\mu \left(\mu + \lambda\right)}{2\mu + \lambda} \,. \tag{64}$$

The dissociation of dislocation pairs, which results in melting at a temperature T_m and is an analogue of the vortex– antivortex dissociation in the standard BKT transition, occurs if [3, 37, 39]

$$k_{\rm B}T_{\rm m} = \frac{Ka_0^2}{16\pi} \,. \tag{65}$$

Halperin and Nelson [37, 38] and Young [39] derived equations that include the renormalization of the moduli μ and λ due to coupled dislocation pairs. These equations, which are analogues of Eqns (9), have the form

$$\begin{aligned} \frac{\mathrm{d}\mu^{-1}(l)}{\mathrm{d}l} &= 3\pi y^2(l) \exp\left(\frac{K(l)}{8\pi}\right) I_0\left(\frac{K(l)}{8\pi}\right) + O(y^3),\\ \frac{\mathrm{d}\left[\mu(l) + \lambda(l)\right]^{-1}}{\mathrm{d}l} &= 3\pi y^2(l) \exp\left(\frac{K(l)}{8\pi}\right)\\ &\times \left[I_0\left(\frac{K(l)}{8\pi}\right) - I_1\left(\frac{K(l)}{8\pi}\right)\right] + O(y^3), \end{aligned}$$

where $I_0(x)$ and $I_1(x)$ are modified Bessel functions. The quantities K(l) and y(l) are determined from the equations

$$\frac{dK^{-1}(l)}{dl} = \frac{3}{2} \pi y^{2}(l) \exp\left(\frac{K(l)}{8\pi}\right) I_{0}\left(\frac{K(l)}{8\pi}\right) -\frac{3}{4} \pi y^{2}(l) \exp\left(\frac{K(l)}{8\pi}\right) I_{1}\left(\frac{K(l)}{8\pi}\right) + O(y^{3}), \frac{dy(l)}{dl} = \left(2 - \frac{K(l)}{8\pi}\right) y(l) + O(y^{3}).$$
(66)

Here, the fugacity y is of the form $y = \exp \left[-E_c/(k_B T)\right]$. Using the renormalization group analysis of the system described by Hamiltonian (63), several predictions for the parameters characterizing two-dimensional melting were made in Refs [37–39].

$$\frac{a_0^2 K}{k_B T} \simeq \frac{16\pi}{1 - c|t|^{\nu}} , \qquad (67)$$

where $t = (T - T_m)/T_m$, v = 0.3696, and a_0 is the distance to the nearest neighbor. Below the transition point, the correlation function and the structure factor are [38]

$$g_{\mathbf{G}}(r) \propto r^{-\eta_G(T)},$$

$$\eta_G(T) = k_{\mathbf{B}}T |\mathbf{G}|^2 \frac{3\mu_R + \lambda_R}{4\pi\mu_R(2\mu_R + \lambda_R)},$$

$$S(q) \propto |\mathbf{q} - \mathbf{G}|^{-2 + \eta_G(T)},$$
(68)

where μ_R and λ_R are the renormalized Lamé coefficients.

Above the transition point, a finite dislocation density results in an exponential decay of the correlation function: $g_{\mathbf{G}}(r) \propto \exp(-r/\xi_{+}(T))$, where $\xi_{+}(T) \propto \exp(c/|t|^{\vee})$. The heat capacity peaks at temperatures above T_{m} , with the shape of the peak depending on the type of model.

The properties of melting in the BKTHNY model are similar to those of the usual BKT transition. However, Halperin and Nelson [37, 38] noted that a liquid turns out to be nonisotropic above the point of dislocation pair dissociation. They found in [37, 38] that the dislocation pair dissociation does not completely destroy the long-range orientational order and merely transforms it into a quasilong-range one. This can be qualitatively explained by simple estimates [129]: in the presence of a free dislocation, the displacement field is of the form $u \propto \ln L$, where L is the system size, and hence the appearance of dislocation should destroy the long-range translational order. At the same time, the angle of rotation associated with the relevant displacement field, Eqn (57), is $\omega \propto 1/L$, and hence the orientational order should not be completely destroyed.

As the phenomenological orientational order parameter for a triangular lattice, Nelson and Halperin [38] suggested considering the quantity

$$\psi(\mathbf{r}) = \exp\left(6i\vartheta(\mathbf{r})\right),\tag{69}$$

where $\vartheta(\mathbf{r})$ is the orientation of the bond between the two nearest neighbors relative to some fixed axis. At a temperature above $T_{\rm m}$, the quasi-long-range order is characterized by a power-law correlation decay:

$$\langle \psi^*(\mathbf{r})\,\psi(0)\rangle \propto r^{-\eta_6(T)}$$
. (70)

A similar power-law correlation decay should be observable in two-dimensional nematic liquid crystals [130], but the order parameter then has the form $\exp(2i\vartheta(\mathbf{r}))$, which is reflective of the two-fold symmetry of the liquid crystal. In the case of triangular lattice melting, the order parameter has a six-fold symmetry, and therefore the anisotropic phase was termed hexatic.

Disclinations in a solid are strongly bound in dislocations because the interdisclination interaction potential is proportional to the distance squared. But in the hexatic phase, this interaction is screened by free dislocations, resulting in the logarithmic form of the interaction potential [38]. To describe long-wavelength fluctuations in an anisotropic liquid, Nelson and Halperin [38] proposed the phenomenological Hamiltonian

$$H_{\rm A} = \frac{1}{2} K_{\rm A}(T) \int d^2 r \left(\nabla \vartheta(\mathbf{r}) \right)^2, \qquad (71)$$

where the Frank constant $K_A(T)$ is related to η_6 as

$$\eta_6(T) = \frac{18k_{\rm B}T}{\pi K_{\rm A}(T)} \,. \tag{72}$$

With the use of expression (71), it is shown in [38] that the disclination interaction Hamiltonian in the hexatic phase takes the form [cf. expression (6)]

$$H_{\text{disc}} = -\frac{\pi K_{\text{A}}(T)}{36} \sum_{i < j} s(\mathbf{r}_i) s(\mathbf{r}_j) \ln \frac{|\mathbf{r}_i - \mathbf{r}_j|}{a} + E_{\text{cd}} \sum_i s^2(\mathbf{r}_i) ,$$
(73)

where E_{cd} is the disclination core energy, $s(\mathbf{r}) = -1$ for an atom with seven nearest neighbors, and $s(\mathbf{r}) = +1$ for an atom with five nearest neighbors (see Fig. 8).

Disclination Hamiltonian (73) can be brought to the form of expression (6), and therefore all results of the BKT theory for the XY model can be used for describing the hexatic-phase–isotropic-liquid transition that is associated with the dissociation of disclination pairs.

Nelson and Halperin [38] hypothesized that the dissociation of disclination pairs occurs for $T_i > T_m$. The equation for T_i is

$$T_{\rm i} = \frac{\pi K_{\rm A}(T_{\rm i})}{72k_{\rm B}T_{\rm i}} \,. \tag{74}$$

At a temperature $T > T_i$, the Frank constant vanishes in a jumpwise manner. As $T \to T_m$ from above, $K_A(T) \propto \xi_+^2(T)$. The exponent $\eta_6(T_i) = 1/4$. The orientational correlation length behaves as $\xi_6 \propto \exp(b/|T - T_i|^{1/2})$ as $T \to T_i$ from above.

We note that Hamiltonian (71) coincides in form with Hamiltonian (1) of the *XY* model, which evidently results in the coincidence of renormalization group equations and the critical behavior in the vicinity of the phase transition.

Thus, the BKTHNY theory predicts that the melting of two-dimensional lattices can occur by means of two continuous transitions. During the first one, dissociation of dislocation pairs occurs with the formation of an intermediate hexatic phase, which next transforms into an isotropic liquid by means of a second continuous transition, during which the dissociation of disclination pairs occurs.

As mentioned above, the BKTHNY theory involves several significant assumptions. First of all, there is the assumption of a high dislocation core energy, which corresponds to the low activity $y \propto \exp[-E_c/(k_BT)]$, in which the expansion is performed. We can expect that the kind of transition would vary with the core energy E_c . This variation, which is observed in the ordinary BKT theory, was discussed in Section 3.1 [43, 62, 63, 66, 69, 131–133].

Unfortunately, approaches that allow consistent calculations of E_c are so far nonexistent. We also recall that presently there is no theory of the hexatic phase that would include a microscopic expression for the Frank modulus $K_A(T)$ (see, however, Refs [134, 135]). Furthermore, a canonical version of the theory [38, 39] was developed in the simplest case (and, in fact, the only case observable experimentally at that time) of a close-packed triangular lattice. The situation has now changed, which we discuss in Sections 3.6 and 3.7 below. For example, we note different lattice versions discovered in computer [136–146] and real experiments, to which the BKTHNY theory should apply. In particular, discovered in recent experimental papers was a square phase in a thin water film confined between graphene sheets [147], as well as in iron in graphene pores [148]. There are indications of the existence of nontrivial two-dimensional structures in a vortex ensemble in a system of several thin superconducting films [149], in a system with the Hertz potential, which describes twodimensional neutral colloidal ensembles [150], and in deoxyribonucleic acid (DNA) complexes [151].

Renormalization group equations for other types of crystal lattices are presently nonexistent, which significantly complicates the description of their melting.

3.3 Melting as a first-order phase transition

At the same time, there are theories that predict that a twodimensional system melts by means of a single first-order transition with the hexatic phase absent. Chui [152, 153] developed a theory in which the possibility of melting via grain boundary formation was considered. The grain boundaries are dislocation strings, which lead to rotations of one part of the crystal relative to another. Multiple grain boundary production results in crystal melting by means of a first-order transition, which precedes the dissociation of dislocation pairs. The competition between random dislocations and grain boundary production depends on the dislocation density. Chui found a weak first-order transition for a low dislocation density (a high dislocation core energy $E_c/(k_BT) > 2.84$) and a first-order transition for low E_c .

In this connection, we mention the results of disclination system simulations [132]. They suggest that the transition order can change from the BKTHNY type to the first-order transition for the dislocation core energy $E_c/(k_BT) \leq 2.84$. This corresponds to Chui's results as regards the part that states the existence of the crossover core energy. However, for a high dislocation core energy, the melting, at variance with Chui's results [152, 153], is a two-stage process.

Kleinert and Janke [154–156] considered the possibility of simultaneous production of free dislocations and disclinations in the system and showed analytically in the framework of the mean-field theory and with Monte Carlo simulations that melting is a first-order transition in this case. Their model relied on the possibility of representing dislocations as disclination dipoles. This model was proposed by Nelson [157] and came to be known as the Laplacian roughening model (LRM). The LRM was the subject of intensive Monte Carlo studies, and contradictory results were obtained. Janke and Kleinert [158] drew a conclusion that the system should melt by means of a single first-order transition, while Strandburg et al. [132, 159] showed that there are two continuous transitions in the system.

More recently, Kleinert came up with a lattice model that explicitly took the rotational stiffness of the lattice into account. The model was investigated analytically and with the use of the Monte Carlo technique [113, 160–163]. It was shown that there is a critical value α_c of the rotational stiffness: when the rotational stiffness is higher than the critical one, the melting proceeds by means of two contin-

uous transitions, while for $\alpha < \alpha_c$ the system melts via a first-order transition.

A continuous version of the model, which takes the existence of orientational order into account (and is formally equivalent to the model proposed by Kleinert), was considered in Refs [129, 164]. In this case, the result is identical to the previous one for $l > l_c$, but for $l < l_c$ the situation turns out to be more complicated: melting can occur both by a first-order transition and by two continuous transitions, depending on the core energy. In this model, the free energy of a deformed isotropic solid can be represented as

$$F = \frac{1}{2} \int \mathrm{d}^2 r \left(2\mu u_{ij}^2 + \lambda u_{kk}^2 \right) + 2\alpha \int \mathrm{d}^2 r \,\varepsilon_{ij} \varepsilon_{lm} \partial_i u_{jk} \partial_l u_{mk} \,. \tag{75}$$

Here, summation over repeated indices is understood, ε_{ij} is an antisymmetric tensor ($\varepsilon_{ii} = 0$, $\varepsilon_{21} = -1$, $\varepsilon_{12} = 1$), $\partial_i = \partial/\partial r_i$, μ and λ are Lamé coefficients [127], the parameter α characterizes the orientational stiffness of the lattice, and $u_{ij} = 1/2(\partial_i u_j(\mathbf{r}) + \partial_j u_i(\mathbf{r}))$ is the deformation tensor. Using (75), we can present the energy of dislocations and disclinations in the form

$$F^{s} = \frac{\pi}{18} \sum_{i \neq j}^{N} s_{i} s_{j} \left(\frac{K}{8} r_{ij}^{2} \ln \frac{r_{ij}}{a} - 2\alpha \ln \frac{r_{ij}}{a} \right) + E_{c} \sum_{i=1}^{N} s_{i}^{2}$$
$$+ \frac{a_{0}K}{12} \sum_{i=1}^{M} \sum_{j=1}^{N} s_{j} \varepsilon_{mn} b_{n} (\mathbf{r}_{i}) (\mathbf{r}_{i} - \mathbf{r}_{j})_{m} \left(\ln \frac{r_{ij}}{a} + C \right)$$
$$- \frac{a_{0}^{2}K}{8\pi} \sum_{i \neq j}^{M} \left[\mathbf{b}(\mathbf{r}_{i}) \mathbf{b}(\mathbf{r}_{j}) \ln \frac{r_{ij}}{a} - \frac{(\mathbf{b}(\mathbf{r}_{i}) \mathbf{r}_{ij})(\mathbf{b}(\mathbf{r}_{j}) \mathbf{r}_{ij})}{r_{ij}^{2}} \right]$$
$$+ E_{d} \sum_{i=1}^{M} \mathbf{b}^{2}(\mathbf{r}_{i}), \qquad (76)$$

where E_c and E_d are the disclination and dislocation core energies, $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, and

$$K = \frac{4\mu(\mu+\lambda)}{2\mu+\lambda} \,. \tag{77}$$

The first two terms in the right-hand side of (76) describe the energy of interacting disclinations, the third term describes the dislocation–disclination interaction, and the last two terms correspond to the dislocation interaction energy. It can be shown that the energy of a given configuration of disclination and dislocation charges is finite only if

$$\sum_{j} s_{j} = 0, \quad \sum_{j} \mathbf{r}_{j} s_{j} = 0, \quad \sum_{j} \mathbf{b}(\mathbf{r}_{j}) = 0.$$
 (78)

We note that the last term in the right-hand side of (75) does not contribute to the long-range interaction between dislocations (although it does contribute to E_d). It is easily seen that the interaction between dislocations coincides with the dipole–dipole disclination interaction (in this case, the Burgers vector **b** is orthogonal to the vector of the disclination dipole moment **d**: $d_1 = b_2$, $d_2 = -b_1$, $d^2 = b^2$). As mentioned above, a dislocation can be treated as a disclination dipole, and we therefore use the dipole moment **d** instead of the Burgers vector **b** in what follows. Conditions (78) show that a two-dimensional lattice is devoid of free disclinations and disclination dipoles (dislocations). In the low-temperature phase, dislocations can exist only in the form of pairs with a zero Burgers vector and disclinations in the form of strongly coupled quadrupole complexes. With increasing temperature, free dislocations or, directly, free disclinations can appear in the system in accordance with the melting scenarios described above. In the first case, free dislocation charges screen the opposite-sign charges, resulting in a short-range (exponentially decaying) interaction between dislocations. The interaction between disclinations is then modified and, while remaining longrange, increases merely as $\ln r$. The system transforms into an ordinary liquid after the appearance of free dislocations. In the second case, the system transforms into a liquid by means of a single transition. In this case, due to screening, the interaction between disclinations becomes short-range.

In Ref. [129], Hamiltonian (76) was considered in the framework of an approximation similar to the Debye–Hückel approximation in the theory of a two-dimensional Coulomb gas [43]. The two-dimensional melting scenario was shown to depend heavily on the orientational elasticity α , the core energy E_c , and the relative disclination core size $t = r_0/a_0$. It turns out that for $\alpha > \alpha_c = Ka_0^2[9/(4\pi^2) + t^2/16]$, a two-dimensional lattice, in accordance with the results in Refs [113, 160–163], melts via two continuous transitions occurring as a result of the successive dissociation of dislocation and disclination pairs. The transition parameters then coincide with those in the BKTHNY theory. It was shown, in particular, that the dislocation density on the hexatic-phase–ordinary-liquid transition line has the form

$$a_0^2 n_0(T) = \frac{\pi}{108} \,. \tag{79}$$

This value can be compared with the result obtained by computer simulations more recently [165]: $n_0 \approx 1/(22a_0^2)$. We also emphasize that the free-dislocation critical density in (79) is in qualitative agreement with the results obtained in considering vortex lattice melting in high-temperature superconductors [166].

Comparing formulas (74) and (79), we find the expressions for the Frank modulus and the exponent η_6 :

$$K_{\rm A}(T) = \frac{2k_{\rm B}T}{3a_0^2 n_0(T)}, \qquad (80)$$

$$\eta_6(T) = \frac{27a_0^2 n_0(T)}{\pi} \,. \tag{81}$$

As can be seen from relations (80) and (81), as the melting line is approached, $n_0(T) \to 0$, we have $K_A(T) \to \infty$ and $\eta_6(T) \to 0$, which corresponds to the existence of a longrange orientational order in a two-dimensional crystal. Condition (79) for the hexatic-phase-ordinary-liquid transition, as well as the expression for the exponent η_6 , is independent of the interaction details of a concrete system (but depends on the lattice symmetry). The appearance of a free dislocation generates a displacement field $u \propto \ln R$, which destroys the quasi-long-range translational order. However, in this case the emergent rotation angle $\omega \propto 1/R$ and therefore the quasi-long-range orientational order persists until the free dislocation density reaches its critical value (79). We also note that relation (79) allows obtaining an expression for the number of sites of the initial hexagonal lattice per dislocation: $n_0(T)^{-1}/\Delta = 216/(\pi\sqrt{3}) \approx 40$; hence, in the vicinity of the melting line, there is one dislocation for every 40 lattice sites, making the dislocations well-defined defects.

However, crystals can melt by means of not only the two transitions described above but also one transition, whereby disclination complexes dissociate in the system to give rise to free disclinations. Due to screening, the interdisclination interaction becomes short-range. In the presence of disclinations, the displacement field at a long range is of the form $u \propto R \ln R$, and hence the phase into which the crystal transforms is completely disordered. Therefore, disclination melting occurs as a first-order transition.

As shown in Ref. [129], the disclination transition temperature increases with the disclination core energy $E_{\rm c}$ and for some E_c^* exceeds the dislocation transition temperature (65). Therefore, for $E_c < E_c^*$, the melting occurs as a firstorder transition and for $E_c > E_c^*$ as two continuous transitions. In Ref. [129], the energy E_c^* was estimated as a function of α and t. The importance of the defect core energy for determining the transition has been noted in numerous papers on two-dimensional melting simulation (see, e.g., Refs [112, 131, 132]). Unfortunately, no unambiguous value of the defect core energy has been found for a realistic model of interacting particles. Commonly used for the simulations are different lattice representations of elastic Hamiltonian (59) (or Hamiltonian (75) with $\alpha = 0$). Putting t = 3 (a realistic value for the defect core size [167]), for $\alpha = 0$ we find $E \approx 2.24$, where $E = 16\pi E_c^*/(Ka_0^2)$. With the dislocation core energy $\approx 2E$, we arrive at a reasonable agreement with the estimates obtained by simulations [112, 131, 132].

It turns out that there are α^* values at which E_c^* vanishes. For $\alpha < \alpha^*$, it is likely that melting occurs via two continuous transitions (we note that α^* depends on *t*). Also, there are values of t^* for which $E_c^* = 0$, and for $t > t^*$ one would expect a two-stage melting. Unfortunately, we are unaware of either real or computer experiments that investigated the dependence of melting on the defect core size.

It is evident that the model considered is a significant simplification in comparison with real systems. Nevertheless, in our opinion, it permits describing a variety of transitions observed in two-dimensional melting. Considering the melting of concrete systems requires relating the parameters that enter Hamiltonian (75), as well as the defect core energies and the defect size t, to microscopic parameters of the system. Unfortunately, so far this has been possible to achieve only for the Lamé coefficients in elastic Hamiltonian (59). We also note the work by Lozovik and Farztdinov [168, 169], who predicted a first-order phase transition based on their analysis of the anharmonic phonon instability of a two-dimensional lattice.

3.4 Relation with the Landau theory of phase transitions

We consider the simple qualitative picture of two-dimensional melting in the framework of Landau's theory of phase transitions [170–175]. For this, we define the corresponding order parameter.

In an ideal crystal, the single-particle distribution function has the symmetry of the crystal lattice. At the zero temperature, T=0, the local density of the system, which is proportional to the single-particle distribution function, has the symmetry of the two-dimensional crystal lattice and can be expanded in the Fourier series in reciprocal lattice vectors **G**. In this case, the Fourier coefficients are the order parameters for the liquid–crystal transition. For $T \neq 0$, the long-range translational order is smeared by thermal fluctuations. However, for sufficiently low temperatures, the expansion in the Fourier series persists, but the Fourier coefficients acquire a dependence on r:

$$\rho(\mathbf{r}) = \sum_{\mathbf{G}} \rho_{\mathbf{G}}(\mathbf{r}) \exp(\mathbf{i}\mathbf{G}\mathbf{r}) \,. \tag{82}$$

The order parameters $\rho_{\mathbf{G}}(\mathbf{r})$ change only slightly over a distance $\sim G^{-1}$ and have an amplitude and a phase:

$$\rho_{\mathbf{G}}(\mathbf{r}) = \rho_{\mathbf{G}} \exp\left(\mathbf{i}\mathbf{G}\mathbf{u}(\mathbf{r})\right). \tag{83}$$

Here, $\mathbf{u}(\mathbf{r})$ has the meaning of the displacement field in the crystal. In two dimensions, the phase of the order parameter fluctuates most strongly [14], and hence fluctuations of the modulus are not considered below. The displacement field can be decomposed into two components, one of which varies smoothly and corresponds to the phonon field, and the other is singular and corresponds to dislocations and disclinations.

The Landau expansion of the free energy, which takes long-wavelength order parameter fluctuations into account, can be written in the form

$$F = \frac{1}{2} \int d^2 r \sum_{\mathbf{G}} \left[A |\mathbf{G} \times \nabla \rho_{\mathbf{G}}|^2 + B |\mathbf{G} \nabla \rho_{\mathbf{G}}|^2 + C |\rho_{\mathbf{G}}(\mathbf{G} \nabla) \rho_{\mathbf{G}}| \right] + \frac{1}{2} a_T \sum_{\mathbf{G}} |\rho_{\mathbf{G}}|^2 + b_T \sum_{\mathbf{G}_1 + \mathbf{G}_2 + \mathbf{G}_3 = 0} \rho_{\mathbf{G}_1} \rho_{\mathbf{G}_2} \rho_{\mathbf{G}_3} + O(\rho^4) \,.$$
(84)

Substituting formula (83) in expression (84), we easily see that the first term in (84) is the free energy (59) of a deformed solid. In this case, the Lamé coefficients μ and λ are functions of the parameters *A*, *B*, and *C* and are proportional to the squared absolute value of order parameter (82).

Using expansion (84), the melting can be described as follows. For T = 0, there are long-range translational and orientational orders. For T > 0, the long-range translational order is destroyed by smooth phase fluctuations and transforms into a quasi-long-range order characterized by slow power-law decay of the order-parameter correlation function. The long-range orientational order persists, with the shear modulus $\mu \neq 0$. With increasing the temperature, free dislocations that correspond to singular phase fluctuations (vortices) of the order parameter appear in the system. This has the result that the system ceases to resist shear ($\mu = 0$), i.e., it becomes liquid. The temperature T_m at which free dislocations appear in the system is defined by the parameters of the first term in expansion (84) and is the melting temperature.

We emphasize that the order parameter modulus $\rho_{\rm G}$ is determined from the minimum condition for expansion (84) (without taking the first term into account) and does not vanish at the temperature $T_{\rm m}$ and that the quasi-long-range order in the system is destroyed by singular phase fluctuations of the order parameter. The order parameter modulus vanishes at some temperature $T_{\rm MF}$, which can be determined from the equality between the free energies of liquid and solid phases as functionals of the order parameter (or the local density). In terms of expansion (84), the equation $a_T = 0$ corresponds to the absolute instability line of the liquid phase. The temperature $T_{\rm MF}$ corresponds to the transition in the mean field approximation. Two cases are possible: 1) $T_{\rm m} < T_{\rm MF}$, the system melts via two BKT-type transitions with the dissociation of dislocation pairs; 2) $T_{\rm MF} < T_{\rm m}$, the system melts via a first-order transition due to the presence of third-order terms in expansion (84).

The ideas based on the use of expansion (84) led to the development of a microscopic theory of two-dimensional melting-the density functional method in crystallization theory [134, 135, 170, 171, 173-179]. This method has been used to study the melting of a system of hard disks [170, 171], a Coulomb system [170, 171], a vortex lattice in a thin superconducting film [171], and systems with the potential of hard disks to which an attractive well [173, 174] and a repulsive step [175, 176] were added. Reasonable agreement (good for the system of hard disks) with the results of computer simulations was obtained in this case. It was shown that systems with a short-range potential should melt via a first-order transition, while for long-range potentials the quasi-long-range order vanishes due to a BKT-type continuous transition. At the same time, this theory does not permit determining the nature of the liquid phase.

3.5 Effect of disorder on the two-dimensional melting scenario

In real experiments in the investigation of two-dimensional melting, experimental systems typically contain frozen-in random fields of various natures: frozen-in impurities with short-range and long-range potentials, random substrate relief, and a random pinning force that owes its origin to substrate nonuniformity.

From the intuitive standpoint, it is clear that the introduction of disorder acting on the particles should exert different effects on the translational and orientational orders. It is evident that even a small disorder must significantly disrupt the particle arrangement on lattice sites. At the same time, the orientation of vectors pointing to nearest neighbors should not change greatly due to the existence of point defects. Therefore, the translational order is rather easily destroyed by disorder, while its effect on the orientational order should be insignificant. As a result, the crystal-hexaticphase transition temperature should decrease, while the hexatic-phase-isotropic-liquid transition temperature should hardly change. This simple physical picture was corroborated by Nelson in [180, 181], where the Hamiltonian

$$H_{\rm dis} = \frac{1}{2} \int d^2 r \left[2\mu u_{ij}^2 + \lambda u_{kk}^2 - 2\omega \delta c(\mathbf{r}) u_{kk} \right]$$
(85)

was considered. Here, $\delta c(\mathbf{r})$ describes the Gauss-distributed fluctuations of the impurity density and ω is a parameter related to elastic moduli. In this case, the exponent $\eta_G(T)$ has the form

$$\eta_G(T) = \left[k_{\rm B} T \frac{3\mu + \lambda}{4\pi\mu(2\mu + \lambda)} + \frac{\sigma\omega^2}{4\pi(2\mu + \lambda)^2} \right] |\mathbf{G}|^2 , \quad (86)$$

where σ is the root-mean-square deviation for the Gaussian distribution, which describes the probability of realizing a specific disorder configuration. We can see from Eqn (86) that even at T = 0, the presence of impurities has the effect that the quasi-long-range translational order exhibits a power-law decay.

Hamiltonian (85) was studied by the renormalization group method. It turned out that the system should exhibit reentrant melting in the framework of the BKTHNY theory: thermally excited dislocation pairs break under the action of the random impurity potential at low temperatures and the solid becomes unstable at T = 0 [180–182]. At a high impurity density, the solid phase becomes completely unstable. In this



Figure 9. Phase diagram of a two-dimensional system in the presence of disorder (see Ref. [184]). $K^* = Ka_0^2/(k_BT)$ [see Eqn (65)].

case, the hexatic phase turns out to be highly immune to random fields.

But from the physical standpoint, this behavior seems to be very strange. The contradiction was resolved in Ref. [183] on the basis of the continuum model (85) and molecular dynamics simulations. It was shown that reentrant melting is absent at low temperatures. This is explained by the fact that the renormalization group method used by Nelson is valid only at low fugacities, while the system can contain configurations that do not satisfy these conditions. However, at high temperatures, the phase diagram corresponds to the diagrams obtained in Refs [180, 182]. Figure 9 shows the qualitative phase diagram of a two-dimensional disordered system obtained by analytic techniques as well as by molecular dynamics simulations of a colloid system with a long-range dipole–dipole interaction [184].

These results were confirmed in experimental studies of the behavior of paramagnetic colloidal particles with the dipole–dipole interaction [185, 186]. Disorder arises in the system due to the pinning of some particles to the substrate at random positions.

We also note that pinning to the positions corresponding to crystal lattice sites and thereby the elimination of a random set of particles from the dynamics, by contrast, stabilizes the crystal and practically leads to the disappearance of the hexatic phase [187].

As shown in Ref. [182], the behavior of a two-dimensional electron crystal—a Wigner crystal—depends on the kind of impurity. In an anisotropic random field corresponding to substrate inhomogeneity, there is a short-range crystal order only, and the genuinely critical behavior is impossible.

3.6 Experiment and computer simulations

As is easily seen, the interaction potential does not appear in the equations of the BKTHNY theory in explicit form. The only limitations that are inherent in the basic equations are a triangular lattice and a high core energy of topological defects [see, e.g., expression (66)]. In this sense, as noted in the Introduction, the theory appears to be universal, and at the moment of its emergence one might even pose the question of whether all two-dimensional systems should melt in accordance with this scenario. The theory of dislocation melting of two-dimensional lattices gave impetus to a wealth of experimental investigations and to computer simulations aimed at verifying its predictions. These experiments are performed on a wide range of objects, including two-dimensional colloids, electrons on the surface of liquid helium, rare-gas atoms on substrates (in particular, xenon on graphite), two-dimensional granular systems, cylindrical magnetic domains in a thin film, vortex systems in high-temperature superconductors (HTSCs) and thin superconducting films in a magnetic field, dust plasmas, and thin liquid (water) films. The number of these papers is so high that it is impossible to dwell on each of them (see reviews [4, 41, 110–114, 188]), and we only list the main results below.

It is noteworthy that computer simulation studies of the behavior of different systems are performed in order to interpret the results of real experiments and simultaneously to consider model systems with different interaction potentials, in order to elucidate the effect of the form of the potential on the character of melting, which we discuss in detail in what follows.

One of the best-known two-dimensional experimental systems in which two-dimensional melting was observed is a system of electrons above a liquid helium surface. Research was undertaken in this area immediately after the advent of the BKTHNY theory. The electrons are held above a superfluid helium-4 surface by the vertical electric field produced by a capacitor with the positive plate under the liquid helium surface and the forces of repulsion between the electrons and the helium surface. The electron density is rather low, $\rho_{\rm e} \approx 10^8 - 10^9 {\rm ~cm^{-2}}$, and therefore the system is classical. For the Coulomb potential, all properties of the system are functions of a single parameter: $\Gamma =$ $e^{2}(\pi\rho_{\rm e})^{1/2}/(k_{\rm B}T)$. For low values of Γ , the electrons form a liquid; with increasing Γ , they form an electron Wigner crystal. The observations involved studies of the behavior of coupled longitudinal oscillations of the Wigner crystal and capillary waves on the liquid helium surface (ripplons) [111, 189–195]. The Wigner crystal melts at $\Gamma_{\rm M} = 137 \pm 15$, and the experimental data confirm the BKTHNY theory in this case. Unfortunately, these experiments do not provide information about the orientational order of the bonds, i.e., do not permit verifying the predictions about the existence of the hexatic phase.

The results of computer simulations of a two-dimensional system with a Coulomb potential performed by the molecular dynamics [196, 197] and Monte Carlo methods also confirm the BKTHNY theory and agree nicely with experimental data.

Another experimental system used widely for studying the melting of two-dimensional systems is rare gases adsorbed on various substrates, mostly on graphite. The rare-gas monolayer structure is incommensurable with the substrate lattice, because carbon atoms are much smaller than rare-gas atoms, and hence the orientational effect of the substrate can be ignored in some cases [111, 112]. X-ray scattering experiments suggest that the system melts via a continuous transition, at a density of more than one monolayer in the case of argon [199, 200] and krypton [201] on graphite and at a density of more than 0.9 monolayer for xenon [202–204].

X-ray scattering experiments show the existence of a continuous transition to the hexatic phase in the xenon monolayer [205, 206] on graphite with hexagonal substrate symmetry as well as on a weakly interacting silver surface [207].

In the last-mentioned experiment [207], the low-temperature phase was interpreted as hexatic glass produced due to the pinning by grain boundaries and substrate steps.

However, some of these experiments came into conflict with computer simulations and with more recent measurements of heat capacity. To interpret the experiments on studying the behavior of xenon with a density of 1.1 monolayer, computer simulations were performed using the molecular dynamics method [208–210]. It was shown that the observed transition [208–210] was a first-order transition and that the apparently continuous behavior was the result of atomic exchange between the first and second layers. Furthermore, several parameters of the BKTHNY theory obtained in these experiments did not coincide with theoretical predictions [203, 211]. A heat capacity peak typical of a first-order transition was discovered for xenon densities above and below 1 monolayer [212].

Continuous melting of argon on graphite at a density below 1 monolayer was ascertained using X-ray scattering [199] and heat capacity measurements [200]. However, more precise measurements with the use of a higher-homogeneity substrate showed the behavior of heat capacity typical of a first-order transition [213]. Therefore, the experimental data on the behavior of the system of adsorbed rare-gas atoms are apparently an indication that the interpretation in terms of the BKTHNY theory is impossible and suggest a weak firstorder transition [212, 213].

Results important for the explanation of two-dimensional melting were obtained in the study of a model system consisting of polysterene spheres in a liquid between two glass plates. The plates were arranged at a small angle to each other, which permits the density of the system to be continuously changed in space [214, 215]. The behavior of the system could be observed in real time and real space, which offered significant advantages over computer experiments.

The system of equigranular charged polysterene spheres in water, interacting via a screened Coulomb potential, was studied in [214–218] Videomicroscopy was used to study the behavior of the system depending on its density, which increased upon increasing the plate separation. Discovered in these papers was a two-stage melting, which agreed with the BKTHNY theory.

Two systems of polysterene spheres on the surface of water were considered in [219]. The system with 2.88 µm spheres exhibited features of melting in accordance with the BKTHNY scenario, including the existence of the hexatic phase. At the same time, in the system of 1.01 µm spheres, the hexatic phase was absent and the structure of defects in the melting was different from the simple pattern of two-stage melting. The free expansion of the system of water-dispersed 1.01 µm spheres confined between two glass plates was considered in [220, 221]. Although a two-stage melting was observed, the structure of defects was more consistent with a first-order transition, because dislocations clearly formed the grain boundaries. So far, it is unclear whether the differences observed in the melting resulted from problems with equilibrium relaxation in different systems or the reason lies with the difference between the interaction potentials.

In [222], the behavior of 1.9 μ m polysterene spheres was studied in a ferromagnetic liquid confined between two glass plates in a magnetic field that was perpendicular to the plates. The thus produced 'voids' in the ferro-medium interacted via the magnetic dipole–dipole potential. On lowering the field,

the system melted via a first-order transition with the constant value $\Gamma = V(r_s)/(k_BT_m) = 62 \pm 3$, where V(r) is the potential and r_s is the Wigner–Zeits radius. These results are consistent with the data of molecular dynamics simulations [223]. In the experiment in Ref. [222], as well as in the experiment in Ref. [227], the disorder in the system was due to the boundaries of grains inherent in the initial crystal.

The melting in systems of 1.6 and 2.0 µm polysterene spheres interacting via the dipole-dipole potential induced by an external electric field perpendicular to the plane of the system was considered in [228, 229]. In a high field, the system crystallizes. The translational and orientational correlation functions, as well as the critical parameters of the power-law decay of these correlators, agree with the BKTHNY theory. The observed defects correspond to predictions for the crystalline, hexatic, and isotropic phases, but no grain boundary formation was observed. The orientational correlation function exhibits a clear hexatic-to-isotropic phase transition. It is noteworthy that the $\Gamma = 61 \pm 3$ parameter value, at which melting was observed, is in good agreement with the result of computer simulations mentioned above [223], but the transition type does not coincide with the firstorder transition obtained by the molecular dynamics method [197, 223].

Interesting results were obtained by Marcus and Reis, who considered the system of colloidal particles covered by a 'brush' of oligomers. The effective interaction potential is a hard sphere 0.928 μ m in diameter with a 300 Å wide repulsive step added to it. Two first-order transitions were discovered: crystal–hexatic and hexatic–isotropic-liquid transitions. These results are a qualitative confirmation of the results obtained in [225] (see also Ref. [226]).

The most convincing experimental confirmation of the BKTHNY theory was obtained in the series of papers [185, 186, 230–236], which comprised the results of real experiments and of Monte Carlo simulations for particles interacting via a dipole–dipole potential V(r). The authors of these papers considered the system of spherical paramagnetic colloidal particles with the diameter $d = 4.5 \mu m$, which were pressed to the water–air interface by the force of gravity. The interface was formed in a drop 8 mm in diameter, which was formed by the surface tension force in a glass pore closed from above. The magnetic field directed perpendicular to the surface produced a dipole moment in the colloidal particles. The dimensionless interparticle interaction has the form [232]

$$V(r) = \frac{\Gamma}{r^3} , \qquad (87)$$

$$\Gamma = \frac{\mu_0}{4\pi} \frac{\chi^2 H^2(\pi\rho)^3}{k_{\rm B}T} \propto \frac{1}{T_{\rm eff}} \,, \tag{88}$$

where ρ is the density of the system. We can see from Eqn (88) that increasing the magnetic field is equivalent to lowering the temperature. On the drop surface, there are of the order of 100,000 particles, whose coordinates and velocities are determined by videomicroscopy. About 3000 particles fall within the field of view of the objective lens. The information thus obtained allowed calculating the correlation and thermodynamic functions of the system, which were compared with the BKTHNY theory predictions. Remarkable agreement was reached between the theoretical and experimental results. Figure 10 shows the structural factors corresponding to crystalline and hexatic phases and to an



Figure 10. Structural factors of a colloidal system that correspond to (a) crystalline and (b) hexatic phases and to (c) isotropic liquid (borrowed from Ref. [232]).

isotropic liquid, which were obtained by processing experimental data [232].

We also mention Ref. [237], which considered the behavior of a dilute two-component two-dimensional system consisting of $\approx 99\%$ polysterene spheres 2.2 µm in diameter and $\approx 1\%$ of spheres 3.0 µm in diameter, which interacted via a dipole–dipole potential. The system is in the state of hexatic glass, in which dislocations are pinned by larger particles. The transition to the isotropic phase due to melting is consistent with the mechanism of disclination pair dissociation.

Similar results were obtained in the investigation of a system of cylindrical magnetic domains of opposite orientation in a thin film [238–240]. These domains interact via a dipole–dipole potential. The magnetization perpendicular to the film is aligned with the applied magnetic field (is opposite to it in the case of a domain). The system is a hexatic glass at a high magnetic-domain density (large Γ) owing to domain pinning. With decreasing Γ (with increasing the field strength), a continuous transition to an isotropic liquid was observed.

We note that the existence of hexatic glass is consistent with the theoretical analysis in [241], where the author shows that in two-dimensional systems with a microscopic disorder, the crystal-hexatic phase transition is nonexistent and the most-ordered state is hexatic glass (i.e., a hexatic phase whose shear modulus can be nonzero).

The above analysis of experimental data allows concluding that there hardly exists a single scenario of melting in two directions. It is likely that the melting mechanism depends on the specific kind of interparticle interaction, and first-order transitions and a scenario corresponding to the BKTHNY theory are possible in this case. Moreover, it can be inferred with a certain degree of confidence that in the case of longrange (Coulomb and dipole–dipole) potentials, melting occurs by two continuous transitions with an intermediate hexatic phase (the BKTHNY theory). This conclusion was further confirmed by computer simulations. At the same time, it was shown that a more complicated scenario is also possible.

A number of two-dimensional system simulations were performed to verify the theories of two-dimensional melting. These papers are reviewed, for instance, in Refs [4, 41, 110, 112–114, 188, 230, 242]. As stated above, experimental data lead to the conclusion that there is most likely no single scenario of two-dimensional melting. A similar situation also takes place in work involving computer simulations. For example, we mention several papers that confirmed the twostage melting scenario [243–248]. At the same time, the traditional first-order transition was found in the majority of studies [223, 249–258]. Furthermore, one more scenario was proposed in the framework of computer simulations: it was shown that melting can occur via two transitions with an intermediate hexatic phase. In this case, the crystal transforms into the hexatic phase by a continuous **BKT** transition and the hexatic phase transforms into the isotropic liquid by a first-order transition [141, 142, 187, 270, 271, 279–282].

It is noteworthy that two-dimensional system simulations encounter serious difficulties due to strong fluctuations. This has the effect that the characteristic correlation lengths and relaxation times become very long as the melting line is approached, which requires considering systems consisting of a large number of particles, which then have to be thermalized for a very long time to obtain trustworthy data. That is why similar simulation techniques sometimes lead to opposite results even when they are applied to systems with the same potentials.

Different methods are used to determine the transition scenario and its parameters. As follows from Landau expansion (84), determining the melting scenario requires comparing the first-order transition temperature $T_{\rm MF}$ and the temperature $T_{\rm m}$ of instability with respect to free dislocation production. To determine $T_{\rm MF}$, use is made of either the method of constructing common tangents to the Helmholtz free energy [259] or Maxwell's construction for the van der Waals (Mayer–Wood [260]) loops in isotherms. As the number of particles increases, the loops become smoother but do not vanish even for a very large number of particles [266].

A detailed analysis of the behavior of Mayer–Wood loops under variation of the number of particles was performed in Refs [271, 272]. In principle, as shown by the Monte Carlo method using the example of hard disks and the twodimensional Ising model [272], the Mayer–Wood loops are observed in isotherms for a finite number of particles both for systems that exhibit a first-order transition and for systems with a continuous transition. However, these loops behave differently upon increasing the number of particles. For the first-order transition, the loop is present in the two-phase domain and is defined by the surface free energy ΔF of the interface [260]. For a fixed density, the energy per disk $\Delta f = \Delta F/N$, which can be calculated from the equation of state [270], behaves as $\Delta f \propto N^{-1/2}$. At the same time, for a continuous transition, the asymptotic form is $\Delta f \propto N^{-1}$, and the loops in isotherms rapidly smooth out as the number of particles in the system increases.

A similar scaling is illustrated in Ref. [261] by the example of two Potts models with 8 and 10 states, which demonstrate a first-order phase transition. In [271], the behavior of Mayer– Wood loops was analyzed for hard disks with $N = 256^2$, 512^2 , and 1024^2 , which showed that the position of the loops hardly changed, despite the lowering of the height of their maxima. Applying these methods gives the phase diagram that actually represents the thermodynamic stability lines. At temperatures above $T_{\rm MF}$, the crystal phase cannot exist.

We note that when melting occurs in accordance with the BKTHNY scenario, the isotherms also exhibit a nonmonotonic behavior due to the presence of the hexatic phase. However, the Mayer–Wood loops are hardly present for a large number of particles [265].

At the same time, as discussed in relation to Landau expansion (84), there is a temperature $T_{\rm m}$ at which free topological defects (dislocations) appear in the system and the shear modulus vanishes, i.e., the crystal lattice melts. When $T_{\rm m} < T_{\rm MF}$, the system melts via a continuous BKT transition. To determine $T_{\rm m}$, the orientational and translational order parameters, as well as the correlation functions of these parameters are used (see Eqns (91)–(94) in Section 3.7). In this case, the use of the order parameters yields an approximate estimate of the crystal-hexatic transition temperature $T_{\rm m}$ and the hexatic-isotropic-liquid transition temperature T_i , especially if the dependence of the order parameters on the number of particles in the system is taken into account (strictly speaking, in the limit of an infinitely large system, the translational order parameter is equal to zero in the crystalline phase with a quasi-long-range order, while the orientational order parameter is equal to zero in the hexatic phase with an infinitely large number of particles). To obtain information about the system behavior in this case, we should resort to a scaling of the behavior of these parameters by using a sequence of ensembles of increasing size (see, e.g., Ref. [258]). When the system is sufficiently large, however, the use of the order parameters yields reasonable qualitative estimates of $T_{\rm m}$ and $T_{\rm i}$.

To correctly determine the instability points of the crystal and hexatic phases, in our view, it is worth analyzing the asymptotic behavior of the correlation functions of translational and orientational order parameters, while the transition points are to be determined from the conditions that the exponents reach their critical values, $\eta_T(T_m) = 1/3$ and $\eta_6(T_i) = 1/4$. With the scale invariance of these correlation functions in the corresponding phases with quasi-long-range order taken into account, this approach permits obtaining results that are independent of the number of particles in the system, if it is large enough for obtaining correct asymptotic behavior of the correlation functions. A detailed description of the application of this approach to a specific system is given in Section 3.7.

It is pertinent to note that the hexatic phase, as a rule, turns out to be very narrow. In some cases, when there is a first-order hexatic-isotropic-liquid phase transition and a continuous crystal-hexatic phase transition, this can lead to an incorrect determination of the melting scenario. In this connection, promise is shown by the study of melting in the presence of random disorder, which broadens the hexatic phase without changing the melting scenario, while in the case of melting by the first-order transition, it can change the melting scenario as well, as shown in Section 3.7.

The simplest system that exhibits a solid–liquid transition in two dimensions is a system of hard disks, which was studied by computer simulations beginning with the classic papers by Alder and Wainwright [22–25]. By considering the Van der Waals loop in the pressure–density curve, which is often referred to as the Mayer–Wood loop [26], Alder and Wainwright drew a conclusion that melting occurs as a firstorder transition. The reduced densities $\rho\sigma^2$, where σ is the hard-disk diameter, of the coexisting liquid and solid phases were $\rho_f \sigma^2 = 0.880$ and $\rho_s \sigma^2 = 0.912$. These results were confirmed by Hoover and Ree [262], who obtained $\rho_f \sigma^2 =$ 0.878 and $\rho_s \sigma^2 = 0.922$. In these early studies, the system size did not exceed 870 particles and the dependence of the transition on the system size was not explored.

As shown in Ref. [245], the main system parameters, including the shear modulus and the order parameter for orientational bond order, depend heavily on the system size in the vicinity of the melting line. In connection with these dimensional effects, a system of a much greater size, consisting of 16,384 particles, was considered in [241], and the values $\rho_f \sigma^2 = 0.887$ and $\rho_s \sigma^2 = 0.904$ were obtained in this case. In [250], the size dependence of melting for a constant-pressure ensemble was analyzed with the use of the Lee-Kosterlitz scaling method [263] in the framework of the Monte Carlo technique. The results were interpreted as a 'rigorous' proof of the existence of the first-order transition. It is likely that true hydrodynamic equilibrium was reached in the system, but the degree of rigor in the treatment in Ref. [263] was quite illusory, because the system size was much shorter than the correlation length.

A scaling analysis of the orientational order parameter, the susceptibility with respect to this parameter, and the compressibility for large systems (up to 16,384 particles) was performed in [251] and [258]. A first-order transition was obtained in this case and the transition parameter values coincided with the data in Ref. [249]. However, we mention the recent Monte Carlo simulations in [264], with the conclusion that the system melted via one continuous transition, without a hexatic phase, for $\rho\sigma^2 = 0.794$. The cause of disagreement supposedly lies in the difficulty of attaining true thermodynamic equilibrium. A good illustration of this point is provided by the computer simulation classic Kurt Binder [258, 265]. In the first study, a first-order transition in hard disks was discovered, while the melting of this system in the second paper was described by molecular simulations and the renormalization group method as a continuous transition without a hexatic phase.

The melting of a system of hard disks with the number of particles in the Monte Carlo simulations $N = 512^2$, 1024^2 , 2048^2 was considered in [266]. It turned out that the Mayer–Wood loop becomes less pronounced with an increasing number of particles, although even for the greatest values of N, the transition remained a weak first-order one. The transition density was estimated as $\rho = 0.920$ (also see Refs [267–269]). At the same time, a scaling analysis of the orientational correlation function showed that the immediate vicinity of the transition density exhibited a behavior typical of the hexatic phase, although no two-stage transition was found. In recent papers [270, 271], an entirely new view on the melting of hard disks was proposed. We discuss these papers below.

The situation with continuous potential systems turns out to be even more complicated. As shown analytically in [273], for $1/r^n$ potentials, there cannot be a volume jump in the melting for n < d, where d is the spatial dimension. Therefore, in the two-dimensional case, the melting of a system with the Coulomb potential 1/r must occur without a jump in volume. This is consistent with the conclusion in [197], where a system with the 1/r potential was shown to melt via two continuous transitions, and a system with the dipole potential $1/r^3$, via a first-order transition. Studying the systems with $1/r^n$ potentials, $3 \le n \le 6$, leads to the same conclusion [223, 252, 253]. Lastly, we mention Ref. [224] as regards the results of molecular dynamics studies of a system of 780 particles interacting via a soft-sphere potential $1/r^{12}$. In this case, considering the Mayer-Wood loop and comparing the free energies shows that the system melts via a weak first-order transition.

The bulk of early computer simulation results (also see Ref. [112]) led the majority of researchers to the conclusion that systems with a long-range (for instance, Coulomb) potential melt in accordance with the BKTHNY theory scenario, while a short-range potential results in melting by a first-order transition. At the same time, Bagchi et al. [247, 248] showed rather convincingly (with an analysis of scaling effects with even larger systems, up to 65,536 particles) that a system with the $1/r^{12}$ potential melts via two continuous transitions with an intermediate hexatic phase in accordance with the BKTHNY theory. By Monte Carlo simulations of a system with the Lennard-Jones potential and a very large number of particles (over 100,000), the authors of a more recent paper [274] also concluded that melting occurs by two continuous transitions, in accordance with the BKTHNY theory.

As mentioned above, all these discrepancies can be a natural consequence of errors emerging in the simulations of phase transitions. In the vicinity of the phase boundary, the correlation length of the order parameter can be long enough to exceed the system size and thereby lead to false results. In addition, thermodynamic equilibrium is hardly attainable because of long relaxation times, which requires a significant increase in the simulation time for decreasing statistical errors. In the study of a system with the $1/r^{-12}$ potential performed in Ref. [275], it was shown that the result is highly sensitive to the choice of boundary and initial conditions. The scaling dimensional analysis, which was invented for overcoming some of these difficulties [263], is also difficult to apply because of the two diverging correlation lengths corresponding to the orientational bond order and the translational order.

We also note the research on the behavior of Yukawa potential systems, which can be applied, in particular, to dust plasmas [276–278].

In this situation, the appearance of papers by Krauth et al. [270, 271] turned out to be a sensation. Recently, one more melting scenario was proposed in [179, 270, 272] (see also Refs [280, 281, 283]) based on the application of three computer simulation techniques (two versions of the Monte Carlo method and the molecular dynamics method) to large systems (up to 1024² particles) with a subsequent thorough data analysis, which included consideration of the scaling behavior of Mayer–Wood loops in isotherms as well as of the orientational and translational order parameters. It turned out that melting can occur via two transitions. In this case, however, contrary to the BKTHNY theory, the solid–hexatic

phase transition is a continuous BKT type and the hexaticisotropic-liquid phase transition is first order.**

Special mention should be made of Ref. [279], which considered the melting of a system of soft disks described by a $1/r^n$ potential. It was shown that the system melts in accordance with the BKTHNY theory for $n \le 6$ and in accordance with the scenario described above for n > 6 [187, 270, 271, 279–281]. This melting scenario is described in the Conclusions (Section 4).

As shown in Ref. [282], a system with the Hertz potential also melts via two transitions: a continuous crystal-hexatic phase transition and a first-order hexatic-isotropic-liquid transition. It is pertinent to note that the hexatic phase domain in the phase diagram is usually very narrow, which might well be interpreted in computer and real experiments as a simple first-order crystal-isotropic-liquid transition. Quite beneficial in this case is the use of random pinning to broaden the hexatic phase domain and study its properties in greater detail (see Refs [141, 142] as well as Section 3.7).

Shortly after the advent of the BKTHNY theory, it was applied to the melting of a vortex system in thin superconducting films in Refs [284, 285]. The authors of Refs [284, 285] estimated the melting curves of the vortex system by using the previously obtained expressions for the shear moduli of the vortex lattice [286] and BKT melting criterion (65). However, no estimates were made for the hexatic–isotropicliquid phase transition. The existence of melting of the vortex lattice in thin superconducting films was confirmed experimentally in [166, 287–289], with the data interpreted in the framework of the BKTHNY theory.

In Ref. [290], a high-temperature decomposition was used to calculate the free energies of a vortex lattice and a vortex liquid. These energies were shown to be very close, and therefore the lattice melting cannot be a strongly pronounced first-order transition.

Many papers are dedicated to computer simulations of vortex lattice melting. In the analysis of these papers, it should be borne in mind that one more strongly fluctuating order parameter, which is absent from the ordinary two-dimensional lattice, exists in this system: the superconducting electron density (in the Ginzburg–Landau theory). This has the effect that the above-mentioned problem of attaining equilibrium is aggravated in the case of superconducting films, making the resultant findings rather contradictory.

In Ref. [291], the authors proceeded from the Ginzburg– Landau Hamiltonian and showed that lattice melting exists, but did not determine the transition order. In Refs [292–295], the vortex lattice melting was shown to occur via a weak first-order transition. In Ref. [296], lattice melting was found, with the numerical transition parameters being consistent with the BKTHNY theory and the theoretical estimates in Ref. [285]. But no indications of a hexatic phase were found, and a conclusion was eventually drawn that the vortex lattice melting occurred as a weak first-order transition.

^{**} After the preparation of this review, Ref. [313] appeared, reporting on an ingenious experimental confirmation of the findings of Refs [270, 271]. The authors of [313] considered the behavior of a monolayer of 2.79 μ m colloidal particles in a water–ethanol mixture in tilted geometry and determined the equation of state and the existence domains of the liquid, hexatic, and crystal phases. It turned out that the crystal–hexatic phase transition is a continuous BKT transition and the hexatic phase transforms into an isotropic liquid by a first-order transition. It is noteworthy that quantitative agreement with simulation results [270, 271] was obtained in [313].

At the same, we note Refs [297–300], where the authors carried out Monte Carlo simulations of a vortex system in the high-temperature domain and arrived at the conclusion that vortex lattice melting does not occur. It is therefore not only the transition order but also the very existence of vortex lattice melting that remains to be clarified.

We also note experimental papers [301, 302], where a vortex lattice was shown to melt to an isotropic liquid via three transitions, through hexatic and smectic-like phases.

In general, analyzing the results of computer and real experiments allows concluding that a two-dimensional system can melt in accordance with three scenarios, depending on the form of the potential. An ordinary first-order transition can be observed. However, it is most likely that the BKTHNY scenario is realized for long-range potentials. Recently, a new melting scenario has been proposed, according to which the system can melt via two transitions, the crystal-hexatic transition being of a continuous BKTHNY type, and the hexatic-isotropic-liquid transition, which is of the first order.

3.7 Melting of two-dimensional systems with core-softened potentials

We briefly discuss the results of molecular dynamics simulations of a system described by a potential with a negative curvature in the repulsive domain (a core-softened potential). This potential, which has two characteristic lengths [138, 139], is given by

$$U(r) = \varepsilon \left(\frac{\sigma}{r}\right)^n + \frac{1}{2} \varepsilon \left\{1 - \tanh\left[k_1(r - \sigma_1)\right]\right\},$$
(89)

where σ is the potential core diameter, n = 14, and $k_1\sigma_1/\sigma = 10.0$. We consider systems with two diameters: $\sigma_1/\sigma = 1.15$ and 1.35 (Fig. 11).

Potential (89) was earlier proposed to qualitatively describe the properties of phase diagrams of water-like liquids, including the well-known anomalies observed in water [138–142, 303–311]. In the three-dimensional case, the phase diagram of the system described by potential (89) exhibits maxima and minima in the melting curve, structural polymorphism, anomalies of diffusion, structure, and the thermal expansion coefficient observed in water, and a domain with a glass state [303–311]. In the case of two



dimensions, for $\sigma = 1.35$, polymorphism and anomalous behavior also exist, but the anomalies sequence order corresponds to liquid silica rather than water [132–142]. In what follows, we briefly discuss the phase diagrams and nontrivial melting scenarios for potential (89) in the twodimensional case without random disorder and in the presence of random pinning.

The following dimensionless quantities are used in this section: $\tilde{\mathbf{r}} \equiv \mathbf{r}/\sigma$, $\tilde{P} \equiv P\sigma^2/\varepsilon$, $\tilde{V} \equiv V/N\sigma^2 \equiv 1/\tilde{\rho}$, $\tilde{T} \equiv k_B T/\varepsilon$, and $\tilde{\sigma} = \sigma_1/\sigma$. (The tildes are omitted in what follows.)

Systems with the number of particles ranging from 20,000 to 100,000 were investigated by the molecular dynamics technique (Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) package) [312] in NVT (N = const, V = const, T = const) and NVE (N = const, V = const, E = const) ensembles. We considered systems with a defect density of 0.1%; simulations were carried out for 10 pinning particle configurations, over which we performed averaging.

Several methods were used to determine the boundaries of phase transitions. The primary estimate was made on the basis of an analysis of the equations of state. In the case of first-order transitions, isotherms should exhibit Mayer– Wood loops, which are hardly present for continuous transitions for such numbers of particles. The equations of state are reliable in reflecting the transition domains, i.e., the existence domains of two phases, but provide no information about the transition scenario. To determine the exact boundaries of the hexatic phase and the crystal in our calculations, we used the approach proposed for the first time in Ref. [141], dealing with the long-range behavior of the orientational and translational correlation functions of order parameters.

As discussed in Section 3.2 (also see Ref. [38]), the hexatic phase stability boundary can be determined from the condition that the exponent of the orientational correlation function (OCF) is $\eta_6 = 1/4$, while the translational correlation function (TCF) in the crystal-hexatic transition also shows a power-law decay with the exponent $\eta_T = 1/3$. In the presence of pinning, as discovered in our study [141], the TCF envelope as a function of the range exhibits a kink in logarithmic coordinates. After this kink, the criterion of power-law TCF decay applies with the exponent $\eta_T = 1/3$, which is used for determining the crystal stability boundary in the transition to the hexatic phase.

The presence of orientational and translational ordering in the system was estimated by studying the behavior of the corresponding order parameters and their correlation functions.

To estimate the degree of orientational ordering, we used the order parameter

$$\Psi_6(\mathbf{r}_i) = \frac{1}{n(i)} \sum_{j=1}^{n(i)} \exp\left(\mathrm{i}6\theta_{ij}\right),\tag{90}$$

where θ_{ij} is the angle between the vector \mathbf{r}_{ij} that connects the *i*th and *j*th particles and an arbitrary axis. The summation is performed over all nearest neighbors n(i) of the *i*th particle. The neighbors are determined by the Voronoi construction.

Apart from the local order parameter $\Psi_6(\mathbf{r}_i)$, it is useful to introduce a global parameter ψ_6 , which is the system-average of $\Psi_6(\mathbf{r}_i)$:

$$\psi_6 = \frac{1}{N} \left\langle \left\langle \left| \sum_i \Psi_6(\mathbf{r}_i) \right| \right\rangle \right\rangle_{\rm rp}.$$
(91)

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The outer angular brackets $\langle ... \rangle_{rp}$ denote averaging over the configurations that correspond to different pinning center distributions.

Translational ordering in the system was determined from the order parameter

$$\psi_{\rm T} = \frac{1}{N} \left\langle \left\langle \left| \sum_{i} \exp\left(\mathrm{i}\mathbf{G}\mathbf{r}_{i}\right) \right| \right\rangle \right\rangle_{\rm rp},$$
(92)

where \mathbf{r}_i is the radius vector of the *i*th particle and **G** is the reciprocal lattice vector.

The translational correlation function has the form

$$G_{\rm T}(r) = \left\langle \frac{\left\langle \exp\left(i\mathbf{G}(\mathbf{r}_i - \mathbf{r}_j)\right)\right\rangle}{g(r)} \right\rangle_{\rm rp},\tag{93}$$

where $r = |\mathbf{r}_i - \mathbf{r}_j|$ and $g(r) = \langle \delta(\mathbf{r}_i) \, \delta(\mathbf{r}_j) \rangle$ is the radial distribution function. In the crystal phase without frozen-in disorder, in the limit $r \to \infty$, $G_T(r) \propto r^{-\eta_T}$ with $\eta_T \leq 1/3$ [38]. The OCF $G_6(r)$ is defined similarly:

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$$G_6(r)$$
 is defined similarly:

$$G_6(r) = \left\langle \frac{\langle \Psi_6(\mathbf{r}) \, \Psi_6^*(\mathbf{0}) \rangle}{g(r)} \right\rangle_{\rm rp},\tag{94}$$

where $\Psi_6(\mathbf{r})$ is the local orientational order parameter (90). In the hexatic phase, the OCF decays in accordance with a power law: $G_6(r) \propto r^{-\eta_6}$, where $0 \leq \eta_6 \leq 1/4$ [38]. The hexatic phase loses stability on reaching the condition $\eta_6(T_i) = 1/4$.

The situation for $\sigma = 1.15$ is rather simple. As is evident from Fig. 11, the potential is then close to the soft-sphere potential $1/r^{14}$ and the melting scenario is consistent with the scenario proposed in Ref. [279]: the system melts via two transitions, the crystal-hexatic transition being of the continuous BKTHNY type, and the hexatic-isotropic-liquid transition, which is of the first order. The presence of random pinning lowers the crystal-hexatic phase transition temperature but has practically no effect on the hexatic-isotropicliquid transition, thereby broadening the hexatic phase domain [142].

The $\sigma = 1.35$ case is by far more interesting. By plotting a common tangent to the Helmholtz free energy of the crystal and liquid phases [259] and by applying the Maxwell construction to the Mayer–Wood loop, it is possible to calculate the phase diagram corresponding to the assumption that all transitions are of the first order. As discussed above, this phase diagram is the domain of absolute crystal stability. At the same time, the instability to dislocation pair dissociation can emerge at a lower temperature $T_{\rm m}$, which results in melting via a continuous BKT transition. Applying the criteria based on the behavior of the correlation functions of orientational and translational order parameters permits elaborating the melting scenario. Figure 12 shows the phase diagram of the system whose details are explained below.

Figure 13 depicts the equation of state corresponding to Fig. 12a. As is clear from Fig. 13, the equation of state hardly changes in the presence of pinning. The correlation functions of orientational, G_6 , and translational, G_T , order parameters without and with pinning are depicted in Figs 14a, 14b and 14c, 14d. We can see, first, that random pinning has little effect on the behavior of G_6 , while the translational correlation function G_T changes significantly. In particular, in Fig. 14d we see a kink that corresponds to an additional increase in the exponent η_T caused by disorder [see expression (86)]. As is seen in Fig. 13, in the absence of random



Figure 12. (Color online.) Phase diagram of the system with $\sigma = 1.35$. (a) S—square lattice, T—triangular lattice. In the absence of pinning, melting occurs via a first-order transition. On the introduction of random pinning (density: 0.1%), the crystal—hexatic phase transition line shifts to the higher density side, thereby changing the melting scenario and making the crystal—hexatic transition continuous, and the hexatic—isotropic-liquid transition remains a first-order one. (b) Phase diagrams at low densities. From Maxwell's construction and the correlation function behavior, it follows that in the absence of pinning, the melting in the left branch of the phase diagram occurs via a first-order transition and in the right branch, via a continuous crystal—hexatic transition and a hexatic—isotropic-liquid first-order transition. In the presence of pinning, the last-mentioned scenario is realized in both branches.



Figure 13. Equation of state for T = 0.3 without pinning and in the presence of pinning with a density of 0.1%.



pinning, the instability points corresponding to the conditions $\eta_6 = 1/4$ and $\eta_T = 1/3$ are inside the two-phase domain, which testifies to the realization of a first-order transition. At the same time, in the presence of pinning, the crystal becomes unstable at densities that markedly exceed the one at which the two-phase domain is observed, while the density that corresponds to hexatic phase instability remains inside the Mayer–Wood loop. Therefore, random pinning changes the melting scenario in the first-order transition case such that this transition is converted into two: a continuous crystal– hexatic BKTHNY transition and a first-order hexatic– isotropic-liquid transition.

A similar analysis for the low-density domain in the phase diagram (Fig. 12b) shows that in the absence of pinning, melting in the left branch of the phase diagram occurs via a



Figure 15. Diffusion coefficient D without and with pinning with a density of 0.1%.

first-order transition and in the right one, via a continuous crystal-hexatic transition and a first-order hexatic-isotropicliquid transition. In the presence of pinning, the last-described scenario is realized in both branches [141, 142].

Figure 15 shows the behavior of the diffusion coefficient depending on the temperature, which corresponds to Fig. 12b. As we see from the figure, the presence of pinning results in the crystal transformation into a hexatic phase with a diffusion coefficient different from that for either a solid or an isotropic liquid.

We also note that for potential (89), a domain with a nontrivial square symmetry of the crystal lattice was found in the phase diagram. Recently, a structure of this kind was discovered in the experimental investigation of the properties of water confined between two graphene sheets [147].

4. Conclusions

The Berezinskii-Kosterlitz-Thouless theory was developed more than 45 years ago and was at that time a rather unusual approach to the description of phase transitions in systems where no phase transitions could occur according to the theory accepted at the time. Since then, the theory has become a powerful method widely used in the investigation of not only plane magnets and superfluid ⁴He films, which were the primary concern of the pioneering studies [1-3, 30], but also of a broad spectrum of diverse low-dimensional systems. These include superconductors and Josephson junction systems, quasi-two-dimensional systems of ultracold atoms in magnetooptical traps, liquid crystal films, two-dimensional colloids, electrons on the surface of liquid helium, rare-gas atoms on substrates (in particular, xenon on graphite), two-dimensional granular systems, cylindrical magnetic domains in thin films, vortex systems in HTSCs and thin superconducting films in a magnetic field, dust plasmas, and thin films of liquids (including water) (see, e.g., Refs [4, 41]).

Special mention should be made of two-dimensional melting theories, which received a strong impetus from these studies. Among these theories, we select the Berezinskii–Kosterlitz–Thouless–Halperin–Nelson–Young theory [38, 39], which proposes an unconventional scenario of two-dimensional crystal melting via two continuous transitions with an intermediate hexatic phase. This theory spawned a wealth of experimental and theoretical papers, which were partly described above. Today, it can be stated with a high degree of confidence, which relies on experimental (see, e.g., Refs [111, 185, 186, 189–195, 230–236]) and computer simulation [279] data, that systems with a long-range interaction (for instance, Coulomb or dipole–dipole interaction, and soft spheres $1/r^n$ with $n \le 6$) melt in accordance with the BKTHNY theory.

At the same time, the situation with the description of two-dimensional melting remains rather contradictory. As discussed in this review, melting can also occur via a conventional first-order transition or in accordance with a recently proposed scenario according to which the crystal-hexatic phase transition is a continuous BKTHNY transition, while the hexatic-phase-isotropic-liquid transition is a first-order transition. This scenario is supposedly true for some systems with short-range potentials (for instance, for a potential of the form $1/r^n$, it was shown to take place for n > 6).

At present, there are no precise theoretical criteria that permit determining the melting scenario based on the form of the potential. As discussed above, the dominant standpoint in early papers was that systems with a short-range potential melt by a first-order transition, while systems with long-range potentials melt by two continuous transitions with an intermediate hexatic phase in accordance with the BKTHNY theory. However, after the publication of Refs [141, 142, 270, 271, 279, 280], it became clear that the hexatic phase can also exist for short-range potentials, including the case of hard disks. Moreover, as discussed in Section 3.7 (see also Refs [141, 142]), random pinning is capable of changing the melting scenario and transforming the first-order transition into two-stage melting with a continuous crystal-hexatic phase transition and a first-order hexatic-isotropic-liquid phase transition. Therefore, studying the relation between the form of the interparticle potential and the existence of the hexatic phase is an interesting task, which remains to be unambiguously solved.

The first-order hexatic-isotropic-liquid phase transition can be explained by the fact that the core energy of topological defects (disclinations) is rather low (see Fig. 3 and the discussion in Sections 2.1 and 2.2), but it is not clear how this energy and the Frank modulus of the hexatic phase are related to the interparticle potential. Furthermore, it would appear natural to proceed from the universal Landau theory when discussing phase transitions. While a qualitative explanation of the transition from the crystal phase to the hexatic phase or to the isotropic liquid can be obtained from expansion (84), a similar theory for the first-order hexaticisotropic-liquid phase transition is nonexistent. It is still unclear how it can be constructed, considering the symmetry of the corresponding order parameter. In general, the problem of calculating the core energy of a topological defect from the interparticle potential is still a long way from being completely solved.

As already mentioned, the BKTHNY theory was based on the assumption that the crystal structure is triangular. Since then, a wealth of different versions of two-dimensional crystal lattices have been found, which correspond to different, sometimes quite exotic potentials. Adapting the BKTHNY theory to these structures and deriving the corresponding stability criteria for crystal phases are also important problems.

To summarize, there is good reason to emphasize once again that the theory developed by Berezinskii, Kosterlitz, and Thouless more than 45 years ago, which deservedly brought Kosterlitz and Thouless the 2016 Nobel Prize, has thus far been a powerful incentive to study two-dimensional systems of highly diverse natures.

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