Microscopic description of two-stage melting in two dimensions

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(Submitted 9 March 1995)
Zh. Éksp. Teor. Fiz. **108**, 2044–2060 (December 1995)

The melting of a two-dimensional electron crystal and a system of hard disks, and also of a system of vortices in a superconductor, is considered within the scope of the microscopic theory based on the method of the density functional in the theory of crystallization. Estimates are obtained for the instability points of the crystalline and hexatic phases whereby it is shown that the systems with long-range potentials—the two-dimensional electron gas and the system of vortices—melt by means of two continuous transitions, while the system of hard disks melts by means of a first-order transition, but the hexatic phase is absent. © *1995 American Institute of Physics.*

1. INTRODUCTION

The nature of two-dimensional melting has been the subject of intense discussion in the past 20 years.[1] Significant progress in the understanding of melting in two dimensions was achieved after the appearance of the theory of Halperin and Nelson[2] and Young[3] based on the ideas of Kosterlitz and Thouless[4] (KTHNY theory). This theory predicts that in the two-dimensional case the transition can fundamentally differ from melting of bulk three-dimensional systems. It has been shown that the transition between a crystal and an isotropic liquid can take place by means of two continuous transitions corresponding to dissociation of dislocation and disclination pairs, respectively. The low-temperature solid phase is characterized by a power-law falloff of the correlation function of the translational order parameter (quasi-long-range translational order), wherein the system possesses long-range order in the orientation of the local crystallographic axes (orientational order). Dissociation of dislocation pairs gives rise to a phase characterized by the absence of quasi-long-range translational order but possessing quasi-long-range orientational order in which the shear modulus of the new phase μ is equal to zero. This intermediate phase has been termed hexatic. The properties of the hexatic phase are reminiscent of the properties of a nematic liquid crystal, except that the role of the anisotropic molecules is played by hexagonal clusters consisting of a molecule and its immediate environment. In the hexatic phase there exist bound disclination pairs (free dislocations), whose dissociation at some higher temperature T_i leads to a transition of the hexatic phase to an isotropic liquid.

KTHNY theory has been confirmed by experiments investigating the behavior of a system of electrons on the surface of liquid helium,[6] computer simulations of two-dimensional electron systems,[7,8] computer simulations of the behavior of a system of defects in a solid body,[9] and experiments with a system of charged polystyrene spheres[10] (however, it should be noted that in the latter case the visually observable topological defects are quite complicated and do not coincide completely with the simple picture of melting suggested by KTHNY theory).

At the same time, melting of a two-dimensional system can also take place by means of a single first-order transition as in three dimensions. Many theories predict a first-order transition.[11–15] Some of them,[11,15] based on the density-functional method in the theory of melting,[16,17] do not take fluctuations of the order parameter and associated possible melting mechanisms into account, and their ability to predict the order of the transition is therefore problematical. In this regard, when the transition really is a first-order transition and longwave fluctuations do not play a defining role, these theories are capable of giving a good qualitative description of melting. We will return to this question below.

The possibility of describing both two-stage melting and melting by means of a first-order transition by means of one model has been examined by Kleinert *et al.*[18,19] in a series of papers and also by one of the present authors.[20] References 18 and 19 propose a model that considers, in addition to the standard elastic energy, the orientational rigidity of the lattice l. Using the Monte Carlo approach, they showed that as l increases, crossover takes place from melting by means of a first-order transition to two-stage melting by means of transitions of the Kosterlitz–Thouless type. A similar model was examined in detail in Ref. 20, where it was shown that there exists a critical value l_c of the rotational rigidity, above which the system always melts by means of two continuous transitions. For $l<l_c$ (including the standard case $l=0$) the system melts by means of two continuous transitions if the energy of a disclination nucleus E_d is larger than the critical value E_d^*, whereas for $E_d<E_d^*$ melting takes place as a first-order transition. This result agrees with the results of computer simulations of the behavior of systems of defects.[9,21]

A number of experiments investigating the behavior of a system of adsorbed atoms indicate the impossibility of interpreting the transition within the Kosterlitz–Thouless–Halperin–Nelson–Young theory and appear to demonstrate a weak first-order transition.[22] The majority of efforts at computer simulations of two-dimensional melting show that two-dimensional systems with a short-range potential melt by means of a first-order transition (see, for example, Refs. 1 and 23 and the references therein). A study of systems with a potential of the form $1/r^n$, $3\leqslant n\leqslant 6$ leads to a similar conclusion.[8,24]

1063-7761/95/121115-09$10.00

Consequently, one may conclude that the type of melting is mainly determined by the type of potential, where the first-order character of the transition becomes less pronounced with softening of the potential. In Ref. 25 it was shown that for a potential of the form $1/r^n$ in the two-dimensional case the volume cannot change discontinuously during melting for $n<2$. This result suggests that melting of a two-dimensional electron system with an interaction potential of the form $1/r$ can differ significantly from standard three-dimensional melting. It is probable that the system melts by means of continuous transitions for soft potentials of the form $1/r$, but for short-range potentials melting takes place as a first-order transition.

This conclusion may be illustrated by the following simple, qualitative picture (which is far from obvious from theories which consider the behavior of dislocations and disclinations in a solid body[1]). As was mentioned above, there exists an analogy between the hexatic phase and a nematic liquid crystal; however, the role of rodlike molecules is played by hexagonal clusters consisting of a central particle and its nearest neighbors. These clusters can be ordered only if the interparticle interaction is sufficiently long-range to ensure effective interaction between the clusters, i.e., the interparticle interaction should extend out at least a few interparticle distances in order for the hexatic phase to be able to exist. Thus, the hexatic phase is possible in systems with a short-range interaction. However, only a microscopic treatment can show to what extent this qualitative picture corresponds to reality.

In the present paper we present microscopic estimates for the limits of stability of the crystalline and hexatic phases for two systems: a two-dimensional classical system with interactions of the form $1/r$ which describes the behavior of a system of electrons above the surface of liquid helium, and a system of hard disks. Note that these systems are two opposite limiting cases of a $1/r^n$ potential, namely $n=1$ and $n=\infty$. We will also briefly discuss melting of a lattice of vortices in two-dimensional superconductors, the interaction potential between which is long-range, but differs from the simple $1/r$ form. A brief exposition of some of the results presented here was given in Ref. 26.

2. MICROSCOPIC DESCRIPTION OF SYSTEM PARAMETERS

First we define the order parameters which we will need to describe the transitions.

At $T=0$ the local density of the system, proportional to the single-particle distribution function, has the symmetry of a two-dimensional crystal lattice and can be expanded in a Fourier series over the vectors of the inverse lattice $\mathbf{G}$, where the Fourier coefficients are the order parameters for the liquid–crystal transition. At $T\neq 0$ the long-range order is washed out by thermal fluctuations, and for low enough temperatures the Fourier series expansion is preserved, but the Fourier coefficients acquire a dependence on $\mathbf{r}$:

$$\rho(\mathbf{r})=\sum_{\mathbf{G}} \rho_{\mathbf{G}} e^{i\mathbf{G}\mathbf{r}}.$$

The order parameters $\rho_{\mathbf{G}}(\mathbf{r})$ vary weakly over distances of order G^{-1} and have an amplitude and phase:

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

Here $\mathbf{u}(\mathbf{r})$ has the meaning of a displacement field in the crystal. In two dimensions the phase of the order parameter fluctuates the most strongly,[27] so in what follows we will not consider fluctuations of the magnitude. The displacement field can be expanded into two parts, one of which varies smoothly and corresponds to a background field while the second is singular and corresponds to the dislocations and disclinations.

In terms of these order parameters melting can be described in the following way: at $T=0$ long-range translational and orientational order exists. For $T>0$ the long-range translational order in the system is destroyed by the smooth phase fluctuations and is converted into a quasi-long-range order, characterized by a slow power-law falloff of the correlation function of the order parameter, while the long-range orientational order in the system is preserved and the shear modulus satisfies $\mu\neq 0$. As the temperature in the system is increased there appear free dislocations, corresponding to singular fluctuations (vortices) of the phase of the order parameter. The appearance of free dislocations means that the system ceases to offer any resistance to shear ($\mu=0$), i.e., it becomes a liquid. The temperature T_m at which free dislocations appear is the melting temperature. It should be emphasized that the absolute value of the order parameter does not vanish at T_m, but the quasi-long-range order in the system is destroyed by the singular fluctuations of the phase of the order parameter. The absolute value of the order parameter goes to zero at some temperature T_{MF}, which can be determined by equating the free energies of the liquid and solid phases as functionals of the order parameter (or the local density). These functionals do not take account of the fluctuations of the order parameter, so the temperature T_{MF} corresponds to a transition in the mean field approximation. Two cases are possible: 1) $T_m<T_{\mathrm{MF}}$, the system melts by means of two continuous transitions of Kosterlitz–Thouless type; 2) $T_{\mathrm{MF}}<T_m$, the system melts by means of a first-order transition. (Note that it is specifically the temperature T_{MF} that was considered in the theory of Ramakrishnan[11] as the melting temperature of a two-dimensional crystal.)

To obtain the free energy of the solid phase as a functional of the local density, we use the density functional method in the theory of crystallization.[16,17] In the contemporary version of this method the properties of the initial system are included in the theory via a two-particle direct correlation function (or the statistical structure factor) of the isotropic liquid.[28] The majority of current applications of the density functional method[16] use a simple parametrization of the local density $\rho(\mathbf{r})$ as a sum over the lattice:

$$\rho(\mathbf{r})=\sum_{i=1}^{N} \varphi(\mathbf{r}-\mathbf{R}_i), \qquad (1)$$

where the function $\varphi(\mathbf{r})$ describes the density distribution in the vicinity of the site $\mathbf{R}_i$, and $\varphi(\mathbf{r}-\mathbf{R}_i)$ is chosen in the form of a spherically symmetric Gaussian distribution:

$$\rho(\mathbf{r})=\sum_{i=1}^{N}(\alpha/\pi)\exp[-\alpha(\mathbf{r}-\mathbf{R}_i)^2]. \tag{2}$$

This function is in good agreement with the single-particle density obtained in a computer simulation even for a strongly anharmonic system of hard disks. The parameter α is the localization parameter: the case $\alpha=0$ corresponds to the limit of a homogeneous, isotropic liquid, and an increase in α corresponds to greater localization of the particles relative to the lattice sites. Taking the Fourier transform of Eq. (2), we obtain an expression for the absolute value of the order parameter:

$$\rho_G=\rho\exp(-G^2/4\alpha), \tag{3}$$

where $\rho=(1/V)\int d\mathbf{r}\rho(\mathbf{r})$ is the average density of the system. To calculate the free energy F, we make use of a simple but accurate effective-liquid approximation.[29] In this approximation the difference between the free energy of a solid body and a liquid with the same density, ΔF, has the form ($\beta=1/k_BT$):

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

where $c^{(2)}(r;\hat{\rho}_{\mathrm{ELA}})$ is the pairwise direct correlation function of the "effective" liquid with density $\hat{\rho}_{\mathrm{ELA}}$, which corresponds to a solid body with mean density ρ. Here the effective density $\hat{\rho}_{\mathrm{ELA}}$ is chosen so that the direct correlation function (structure factor) of the effective liquid optimally models the direct correlation function of the solid body. To achieve this result, $\hat{\rho}_{\mathrm{ELA}}$ is defined by the condition that the position of the first peak of the static structure factor of the effective liquid should coincide with the smallest inverse lattice vector of the solid body with mean density ρ. (Recall that the static structure factor $S(q)$ is related to the Fourier transform of the direct correlation function $\tilde{c}^{(2)}(q)$ by the relation (see, for example, Ref. 30) $S(q)=(1-\tilde{c}^{(2)}\times(q))^{-1}$.) The effective liquid approximation has been employed to study crystallization of various three-dimensional systems, in which good qualitative and quantitative agreement with the results of computer simulations were obtained.[16,28]

The localization parameter α is defined by the condition that ΔF have a local minimum with respect to α, and the temperature T_{MF} is defined by the condition $\Delta F=0$ at α corresponding to the minimum of the free energy.

The intensity of the interaction of the dislocations in the lattice is equal to the following dimensionless quantity (see, for example, Refs. 2 and 4):

$$K=\frac{4\mu(\mu+\lambda)}{2\mu+\lambda}\frac{a_0^2}{k_BT}, \tag{5}$$

where μ and λ are the ordinary Lamé coefficients and a_0 is the lattice constant. According to KTHNY theory, K decreases with increase of temperature until it reaches the value 16π, at which the system becomes instable with respect to the formation of free dislocations. In this case the shear modulus μ (and thus K) vanishes abruptly and the lattice melts into the hexatic phase. We denote the temperature at which this occurs as T_m, and the equation for it has the obvious form[2,4]

$$K(T_m)=\frac{a_0^2}{k_BT_m}\frac{4\mu(T_m)(\mu(T_m)+\lambda(T_m))}{2\mu(T_m)+\lambda(T_m)}=16\pi, \tag{6}$$

where $\mu(T)$ and $\lambda(T)$ are the Lamé coefficients, renormalized to take account of bound dislocation pairs. In order to use Eq. (6), it is necessary to know the microscopic expressions for the nonrenormalized Lamé coefficients. These expressions were obtained by the authors of Ref. 31 by comparing the long-range behavior of the correlator of the order parameter, calculated with the help of a phenomenological expression for the elastic energy,[2] with the asymptotic behavior of the analogous correlator obtained from the statistical mechanical equation for the pairwise distribution function. For short-range potentials, expressions were obtained in Ref. 31 for the elastic moduli which correspond to fluctuations with wave vector equal to the smallest inverse lattice vector. Generalization to the case of an arbitrary number of inverse lattice vectors leads to the following expression for the Lamé coefficients:

$$\mu=\frac{k_BT}{16\rho}\sum_G\rho_G^2m_GG^2(\gamma_G+2\delta_G), \tag{7}$$

$$\lambda=\frac{k_BT}{16\rho}\sum_G\rho_G^2m_GG^2(\gamma_G-6\delta_G)+k_BT\rho(1-\rho\tilde{c}^{(2)}(0)), \tag{8}$$

where

$$\gamma_G=2\pi\rho\int r^3dr\,c^{(2)}(r;\hat{\rho})J_0(Gr), \tag{9}$$

$$\delta_G=2\pi\rho\int r^3dr\,c^{(2)}(r;\hat{\rho})J_1(Gr)/(Gr), \tag{10}$$

$J_0(x)$ and $J_1(x)$ are the Bessel functions, and m_G is the number of inverse lattice vectors having the same length.

In the case of the long-range Coulomb interaction, an additional term arises in the elastic Hamiltonian,[32] which makes the effective modulus λ diverge, $\lambda=\infty$, but the expression for μ remains constant and is given by Eq. (7). In this case the expression for K takes the form

$$K=4\mu a_0^2/k_BT. \tag{11}$$

Let us now determine the order parameters and microscopic expressions for the quantities characterizing the properties of the hexatic phase. To determine the order parameters of the hexatic phase, we consider the two-particle conditional distribution function $F_2(\mathbf{r}_1|\mathbf{r}_0)=F_2(\mathbf{r}_1,\mathbf{r}_0)/F_1(\mathbf{r}_0)$, which determines the probability of finding a particle in the vicinity of the point $\mathbf{r}_1$ if the other particle is fixed at the point $\mathbf{r}_0$. Here $F_2(\mathbf{r}_1,\mathbf{r}_0)$ and $F_1(\mathbf{r}_0)$ are the two-particle and one-particle distribution functions, respectively. In a homogeneous, isotropic liquid $F_1(\mathbf{r})\equiv 1$, $F_2(\mathbf{r}_1,\mathbf{r}_0)=g(|\mathbf{r}_1-\mathbf{r}_0|)$, where $g(r)$ is the radial distribution function. Let $\mathbf{r}_1$ and $\mathbf{r}_0$ be the position vectors of nearest neighbors: $\mathbf{r}_1-\mathbf{r}_0=\mathbf{a}_0$. With the appearance of long-range order, the isotropy of the two-particle distribution function is destroyed in the direction of the bonds $\mathbf{a}_0$ (by a bond here we understand a vector joining a particle with one of its nearest neighbors). We write the anisotropic part of the two-particle distribution function $F_2(\mathbf{r}_1,\mathbf{r}_0)$ in terms of $f(\mathbf{r}_1|\mathbf{r}_0)$:

$$F_2(\mathbf{r}_1\mathbf{r}_0)=g(|\mathbf{r}_1-\mathbf{r}_0|)(1+f(\mathbf{r}_1|\mathbf{r}_0)). \qquad (12)$$

The function $f(\mathbf{r}_1|\mathbf{r}_0)$ has the symmetry of the local environment of the molecule at $\mathbf{r}_0$ and in the two-dimensional case can be written in the form

$$f(\mathbf{r}_1|\mathbf{r}_0)=f(a_0,\mathbf{r}_0,\varphi),$$

where the angle φ defines the direction of the vector $\mathbf{a}_0$. The function $f(a_0,\mathbf{r}_0,\varphi)$ can be expanded in a Fourier series:

$$f(a_0,\mathbf{r}_0,\varphi)=\sum_{m=-\infty}^{\infty} f_m(a_0,\mathbf{r}_0)e^{im\varphi}. \qquad (13)$$

The Fourier coefficients $f_m(a_0,\mathbf{r}_0)$ are the order parameters of the anisotropic phase. They vary slowly with $\mathbf{r}_0$ and have amplitude and phase

$$f_m(a_0,\mathbf{r}_0)=f_m e^{im\omega(\mathbf{r}_0)}. \qquad (14)$$

As in the case of the single-particle distribution function, it is possible to neglect the amplitude fluctuations in comparison with the phase fluctuations. In the case of the hexatic phase the main order parameter corresponds to $m=\pm 6$, and we limit ourselves to these values in expansion (13).

The hexatic phase is described by the phenomenological Hamiltonian:[2]

$$H=\frac{1}{2}K_A(T)\int d^2r_0|\nabla\omega(\mathbf{r}_0)|^2, \qquad (15)$$

where $K_A(T)$ corresponds to the Franck constant in liquid crystals. The angle $\omega(\mathbf{r}_0)$, which defines the direction of the bonds, can be represented in the form of a sum of two terms,[2] one of which corresponds to the slowly varying field of the order parameter, and the other to the singular field of topological defects or ensemble of disclinations. Here $K_A(T)$ serves as a measure of the interaction between the disclinations in the hexatic phase. The disclination pairs dissociate at the temperature T_i, at which the Franck constant $\overline{K}_A(T)$, renormalized for the bound disclination pairs, vanishes discontinuously. The equation for T_i has the form[2,20]

$$\overline{K}_A(T_i)=\frac{72k_BT_i}{\pi}. \qquad (16)$$

It can be seen from this equation that to determine the transition temperature T_i it is necessary to know the value of the renormalized coupling constant $\overline{K}_A(T)$, which can be obtained by solving the Kosterlitz–Thouless renormalization group equations with the microscopic expression $K_A(T)$ as the initial value. We have proposed a method of calculating this quantity in a recent paper,[31] based on comparing the long-range behavior of the correlation function of the order parameter (14), calculated with the help of the phenomenological Hamiltonian (15), with the asymptotic behavior of the solution of the microscopic equation for the four-particle distribution function. The expression for the Franck constant $K_A(T)$ has the form[31]

$$K_A(T)=648k_BTa_0^2|f_6|^2[\Gamma_6(a_0,a_0)-(1/2)(\Gamma_5(a_0,a_0)+\Gamma_7(a_0,a_0))],$$

$$\Gamma_m(r_1,r_2)=\frac{1}{2\pi}\int_0^{2\pi}d\varphi\Gamma(r_1,r_2,\varphi)e^{-im\varphi}, \qquad (17)$$

where $a_0^2=2/\sqrt{3}\rho$. The function $\Gamma(r_1,r_2,\varphi)$ was introduced in our earlier papers,[33,34] which addressed orientational ordering of the bonds in simple liquids, and has the form

$$\Gamma(r_1,r_2,\varphi)=\sum_{k\geqslant 1}\frac{\rho^k}{(k-1)!}\int S_{k+1}(\mathbf{r}_1,\ldots,\mathbf{r}_{k+1})g(|\mathbf{r}_3-\mathbf{r}_0|)\ldots g(|\mathbf{r}_{k+1}-\mathbf{r}_0|)d^2r_3\ldots d^2r_{k+1}, \qquad (18)$$

where $S_{k+1}(\mathbf{r}_1,\ldots,\mathbf{r}_{k+1})$ is the sum of irreducible Mayer diagrams of order $k+1$, $r_1=|\mathbf{r}_1-\mathbf{r}_0|$, $r_2=|\mathbf{r}_2-\mathbf{r}_0|$, and φ is the angle between the vectors $\mathbf{r}_1$ and $\mathbf{r}_2$.

To obtain an approximation for $\Gamma(r_1,r_2,\varphi)$, we expand the function (18) in a functional Taylor series in powers of $h(r)=g(r)-1$:

$$\Gamma(r_1,r_2,\varphi)=\rho\left(c^{(2)}(|\mathbf{r}_1-\mathbf{r}_2|)+\sum_{n=1}^{\infty}\frac{\rho^n}{n!}\int c^{(n+2)}\times(\mathbf{r}_1,\ldots,\mathbf{r}_{n+2})h(|\mathbf{r}_3-\mathbf{r}_0|)\ldots h(|\mathbf{r}_{n+2}-\mathbf{r}_0|)d^2r_3\ldots d^2r_{n+2}\right). \qquad (19)$$

Dropping terms with $n\geqslant 3$ in the expansion (19), we obtain

$$\Gamma(r_1,r_2,\varphi)=\rho c^{(2)}(|\mathbf{r}_1-\mathbf{r}_2|). \qquad (20)$$

Note that the approximation (20) corresponds to the well-known hyperchain approximation in classical statistical mechanics.[30] In this approximation, Eq. (17) has the form

$$K_A(T)=648k_BTa_0^2|f_6|^2\rho[c_6(a_0,a_0)-(1/2)(c_5(a_0,a_0)+c_\gamma(a_0,a_0))], \qquad (21)$$

where

$$c_m(a_0,a_0)=\frac{1}{2\pi}\int_0^{2\pi}d\varphi c^{(2)}(\sqrt{2}a_0(1-\cos\varphi)^{1/2};\hat{\rho})e^{-im\varphi}.$$

To obtain an equation for the absolute value of the order parameter, we make use of the exact equation for the conditional two-particle distribution function $F_2(\mathbf{r}_1|\mathbf{r}_0)$, which has the form[33,34]

$$\frac{\rho F_2(\mathbf{r}_1|\mathbf{r}_0)}{z}=\exp\left\{-\beta\Phi(\mathbf{r}_1-\mathbf{r}_0)+\sum_{k\geqslant 1}\frac{\rho^k}{k!}\int S_{k+1}(\mathbf{r}_2,\ldots,\mathbf{r}_{k+1})F_2\times(\mathbf{r}_2|\mathbf{r}_0)\ldots F_2(\mathbf{r}_k|\mathbf{r}_0)d\mathbf{r}_2\ldots d\mathbf{r}_{k+1}\right\}, \qquad (22)$$

where z is the activity. Substituting expression (12) in Eq. (22) and employing the normalization condition

$(1/V)\int F_2(\mathbf{r}_1|\mathbf{r}_0)d\mathbf{r}_1=1$, within the framework of the hyperchain approximation we obtain the following equation for the absolute value of the order parameter f_6:

$$f_6=\frac{\int_0^{2\pi}d\varphi\cos 6\varphi\exp[12c_6(a_0,a_0)\cos(6\varphi)f_6]}{\int_0^{2\pi}d\varphi\exp[12c_6(a_0,a_0)\cos(6\varphi)f_6]}. \qquad (23)$$

As in the case of the standard theory of the density functional, this equation corresponds to the minimum of the free energy functional.

3. MELTING OF A TWO-DIMENSIONAL CLASSICAL WIGNER CRYSTAL

Let us now consider melting of a two-dimensional electron crystal. To investigate the properties of this system, it is convenient to introduce the dimensionless parameter $\Gamma=\sqrt{\pi\rho}e^2/k_BT$, which characterizes the ratio of the mean kinetic energy to the mean potential energy and completely determines the statistical properties of the system. Using the parameter Γ corresponds to a rescaling of length: $\mathbf{r}'=(E^2/k_BT)^{-1}\mathbf{r}$. In the reduced units the average density is $\rho=\Gamma^2/\pi$.

The existence of the Wigner crystal was first demonstrated experimentally by Grimes and Adams,[5] who considered a system of electrons on a surface of liquid helium, where the electron density is so low that exchange effects can be neglected and the system can be treated as purely classical. They showed that a Wigner 2D crystal melts at $\Gamma_m^{\exp}=137\pm 15$. All later experimental results for this system[6] lie in this interval. These results have been discussed theoretically by a number of authors[7,8,14,35,36] who have obtained fair agreement with experiment by taking account of the renormalization of the elastic constants μ and λ due to the background anharmonicity and the bound dislocation pairs and by using the Kosterlitz–Thouless criterion (6). However, the criterion (6) in principle determines only an upper bound on the transition temperature and does not exclude the possibility of a first-order transition at a temperature below T_m. More convincing arguments in favor of the possibility of melting by means of two continuous transitions can be obtained from an analysis of the stability of the hexatic phase. Note that a microscopic expression for the Franck modulus of the hexatic phase was obtained only recently by the authors,[31] so that estimates for hexatic phase–isotropic liquid transitions are absent in the literature with the exception of preliminary results obtained in Ref. 51 for a system of vortices in a two-dimensional superconductor. In the present paper we have undertaken an effort to obtain estimates of the melting parameters and of the hexatic phase–isotropic liquid transition for a two-dimensional classical system of electrons using Eqs. (7) and (21).

In order to use Eqs. (7) and (21), it is necessary to have an expression for the direct correlation function $c^{(2)}(r';\rho)$. Unfortunately, exact analytic results for the function $c^{(2)}\times(r';\rho)$ do not exist at the present time; therefore, in the present work we assume a simple approximation for the direct correlation function which is constructed in the following way: we take the long-range behavior of the approximate function to coincide with the first term of the high-temperature expansion of the exact direct correlation function, i.e., in the reduced units r' the long-range behavior of $c^{(2)}(r';\rho)$ has the form

$$c^{(2)}(r';\rho)=-\frac{1}{r'}. \qquad (24)$$

The direct correlation function is finite for all r'; therefore, in order to model its short-range behavior we assume that an effective diameter d_{eff} exists such that $c^{(2)}(r';\rho)$ is continuous at $r'=d_{\text{eff}}$, has the form (24) for $r'>d_{\text{eff}}$, and can be written for $r'<d_{\text{eff}}$ in the form

$$c^{(2)}(r';\rho)=\bar{c}(r';\rho)+(-\bar{c}(d_{\text{eff}};\rho)-1/d_{\text{eff}}), \qquad (25)$$

where $c^{-}(r';\rho)$ is a function which is finite at $r'=0$. The exact form of the function $\bar{c}(r';\rho)$ is unknown and is chosen on the basis of additional considerations although, as will be shown below, the results depend only slightly on the behavior of the direct correlation function in the region of small r'. In the spirit of the effective liquid approximation[17,29] the effective diameter d_{eff} is defined by the condition that the position of the first peak of the static structure factor coincide with the smallest inverse lattice vector. The position of the first peak of the structure factor is determined mainly by the short-range part of the direct correlation function (25), while the height of this peak is determined by the long-range part. By virtue of this, thanks to the effective liquid approximation, the melting parameters of a classical electron system should depend rather weakly on the exact form of the short-range part of the direct correlation function $\bar{c}(r';\rho)$.

In order to carry out actual calculations, in analogy with the mean sphere approximation we take $\bar{c}(r';\rho)$ in the form of the direct correlation function $c_{HS}^{(2)}(r';\rho)$ for a system of hard disks of diameter d_{eff}. The physical meaning of this choice is that at the given temperature most of the particles cannot approach one another closer than by some distance less than d_{eff}, by virtue of which it may be assumed that the direct correlation function of a system of electrons is well approximated by a combination of two parts, one of which corresponds to the long-range part of the potential and is given by formula (24), and the other, to the presence of a "quasirigid" core, whose diameter depends on Γ.

For $c_{HS}^{(2)}(r';\rho)$ we use the approximate analytic expression obtained in Refs. 15 and 39:

$$\begin{aligned}
c_{HS}^{(2)}(x,\eta)&=-[\partial(\eta Z(\eta))/\partial\eta]\Theta(1-x)[1-a^2\\
&\quad+a^2\eta\omega_2(x/a)],\\
\omega_2(x)&=\frac{2}{\pi}[\arccos x-x(1-x^2)^{1/2}],\\
Z(\eta)&=\frac{1+c_2\eta^2}{(1-\eta)^2},\\
a&=\frac{2+\eta\alpha_2(\eta)}{1+\eta+\eta\alpha_2(\eta)},
\end{aligned} \qquad (26)$$

where $c_2=0.128$, $\alpha_2(\eta)=-0.2836+0.2733\eta$, and $\eta=\pi\rho d_{\text{eff}}^2/4$.

In this case the mean-field thermodynamic instability $\Delta F=0$ (see Eq. (4)) sets in at $\Gamma_{\text{MF}}=21.62$. This value is much lower than the values of Γ experimentally observed and also obtained by computer simulation. Thus, one may expect that the picture of melting of a two-dimensional system of electrons differs from the standard first-order transition corresponding to the condition $\Delta F=0$. Note that precisely this value of Γ would have been obtained from Ramakrishnan's theory[11] (or the analogous theories set forth in Refs. 17 and 15) if they had been applied to a description of the melting of a classical 2D Wigner crystal.

Invoking the Kosterlitz–Thouless criterion (6) and Eqs. (7) and (11), we obtain $\Gamma_m^{\mathrm{KT}}=80.07$. Equation (7) allows one to estimate the renormalization of the shear modulus μ due to the background anharmonicity. The ratio of $\mu(T)$ at the melting temperature to the shear modulus at zero temperature, $\mu(0)=0.245065e^2\rho^{3/2}$ (see, for example, Ref. 7), has the form $\mu(T)/\mu(0)=0.98$. This value is greater than that obtained by other authors[7,14,36] who have studied the influence of phonon–phonon interactions on the shear modulus. In our view, this discrepancy is a result of the approximation (24) for the long-range part of the direct correlation function, which leads to the result that the long-range part is extremely "rigid." One possible way of correcting this result is to use the ring approximation, which is well known in statistical plasma physics, to calculate the long-range part of the direct correlation function. In this case the long-range part of the direct correlation function "softens," which should reduce the ratio $\mu(T)/\mu(0)$ and increase Γ_m^{KT} at the transition point.

In order to demonstrate the stability of the results with respect to the choice of the form of the function $\bar{c}(r';\rho)$, let us consider the simple "rectangular" approximation for this function: we assume $\bar{c}(r';\rho)=-1/d_{\mathrm{eff}}$ at $r'\leq d_{\mathrm{eff}}$, for which the long-range part of the direct correlation function is given by expression (24). In this case $\Gamma_m^{\mathrm{KT}}=79.6$. Thus, variation of the form of the short-range part of the direct correlation function leads to an insignificant change in the transition parameters. As was already mentioned, such stability is to a significant extent the result of using the effective-liquid approximation. Of course, the above considerations do not rigorously prove that the magnitude of the melting parameters depends weakly on the unknown exact form of the short-range part of the direct correlation function; however, they can serve as a convincing illustration of this fact. Note that, in contrast to the short-range part, the long-range part of the direct correlation function has been determined quite well. Therefore, using other approximations should not lead to a qualitative change in the results.

These results for the melting parameters and the shear modulus μ do not take account of renormalization of μ due to bound dislocation pairs. To estimate this renormalization, we use the renormalization group equations, derived for the case of two-dimensional melting by Halperin and Nelson,[2] and expression (7) as the initial condition. The initial value for the activity $y=e^{-E_c/k_BT}$ can be obtained by using the estimates for the energy of the dislocation nuclei E_c obtained in Ref. 35 for the case $T=0$ and assuming that the energy of the dislocation nuclei decreases due to the background anharmonicity in the same proportion as the shear modulus,[7,35] i.e., $E_c=\bar{C}\mu a_0^2/4\pi$, where $\bar{C}=4.88\pm0.98$. For $\bar{C}=4.0$, we obtain $\Gamma_m=114.22$. Note that this value corresponds to the reduced value of the localization parameter $\hat{\alpha}=\alpha/(e^2/k_BT)^2=43.68$, i.e., the crystalline structure in front of the melting line corresponding to the appearance of free dislocations in the system is well defined. The above value of the parameter Γ_m is lower than the experimental results and results of computer simulations; however, they are in good qualitative agreement, and besides, as was mentioned above, they can be improved by using the ring approximation to calculate the asymptotic behavior of the direct correlation function.

Let us now estimate the instability parameters for the hexatic phase. Using Eqs. (16), (21), and (24), (25), we obtain $\Gamma_i^{\mathrm{KT}}=24.07$. However, this value does not take into account the renormalization of the Franck constant $K_A(T)$ due to bound disclination pairs, i.e., it corresponds to an infinite energy of the disclination nucleus $E_d=\infty$. To estimate this renormalization, one can use the renormalization group equations, analogous to the Kosterlitz equations for the case of a planar magnet.[27] In this case the transition temperature T_i is found from the intersection of the line defined by the initial conditions with the "entering" separatrix of the current diagram of the renormalization group equations. The equation for T_i has the form

$$K_A(T_i)-72k_BT_i/\pi=2\pi K_A(T_i)\exp(-\beta E_d). \qquad (27)$$

Unfortunately, at present there are no microscopic estimates of the energy of the disclination nucleus E_d in the hexatic phase; however, using the Hamiltonian (15), in analogy with the result of Ref. 14 one can obtain an estimate for the energy of the disclination nucleus in the form $E_d=\bar{c}\pi K_A(T)/72$, where $\bar{c}\approx 3$. This value of the energy of the disclination nucleus corresponds to $\Gamma_i=25.86$. Thus, within the framework of the proposed theory we have $\Gamma_m>\Gamma_i$ although decreasing $\bar{c}$ narrows the existence region of the hexatic phase.

To illustrate the stability of the results with respect to the choice of the form of the short-range part of the direct correlation function $\bar{c}(r';\rho)$, as in the melting case, we make use of the "rectangular" approximation for $\bar{c}(r';\rho)$ described above. In this case $\Gamma_i=22.84$ for $E_d=\infty$, i.e., as has already been discussed, the results depend only weakly on the form of the short-range part of the direct correlation function.

4. MELTING OF A SYSTEM OF HARD DISKS

In this section we will briefly discuss melting of a system of hard disks. Beginning with the classic work of Alder and Wainwright[40] it has been assumed that a system of hard disks melts by means of a first-order transition. However, during the entire time since the appearance of Ref. 40 this question has been the subject of intense discussion, and only recently have convincing proofs of this fact been obtained.[23] The application of the density functional method to this problem has yielded good qualitative and quantitative agreement with the results of computer simulations; however, the instability with respect to dissociation of dislocation pairs and the possibility of the existence of the hexatic phase have not been examined.

Using the direct correlation function (26) and the condition $\Delta F=0$ [see Eq. (4)], we obtain $\rho_S=0.933$ for the transition density. This quantity should be compared with the value $\rho_S^{\exp}=0.921$ obtained by computer simulation.[38] Thus, a treatment in the mean field approximation leads to good agreement with the results of computer simulation, which is characteristic of first-order transitions. Using Eqs. (5), (7), and (8), we can calculate the value of the dislocation coupling constant in the lattice K. At the transition point we obtain $K/16\pi=4.797$. This is substantially larger than the value $K/16\pi=1$ at which dissociation of dislocation pairs takes place. Renormalization of the coupling constant K to account for bound dislocation pairs can substantially lower its value; however, using the renormalization group equations and assuming that thermal effects renormalize the energy of the dislocation nucleus by the same factor as K, i.e., $E_c=\bar{c}K/16\pi$, it can be shown that fulfillment of the condition $K(T)=16\pi$ can hold for $\bar{c}\approx 0.996$. This value is much smaller than the value below which, according to various estimates,[1,9,12,21] melting should take place as a first-order transition.

However, an even more convincing argument in favor of the assertion that a system of hard disks melts by means of a single first-order transition is provided by an analysis of the possible existence of the hexatic phase. Invoking Eq. (21), we obtain the result that for a system of hard disks the Franck constant satisfied $K_A(T)<0$ at all densities and, according to the simple physical picture given in the Introduction, the hexatic phase cannot exist in a system of hard disks.

5. MELTING OF A VORTEX LATTICE IN A TWO-DIMENSIONAL SUPERCONDUCTOR

In this section we will discuss melting of a vortex lattice in a two-dimensional superconductor according to the theory presented above. Melting of a vortex lattice has been the subject of intense discussion in recent years; however, up to the present time there is no single point of view on the nature of melting in this system. In a number of papers (see, for example, Refs. 51, 41–43) it was assumed that the system melts by means of two continuous transitions in accordance with the KTHNY theory. At the same time, the authors of Refs. 44 and 45 come to the conclusion that the transition can be first-order, but close to second. We also note Refs. 46 and 47, whose authors, on the basis of a Monte Carlo simulation of a system of vortices in the high-temperature region, came to the conclusion that a vortex lattice does not melt. Thus, not only the type of the transition, but even the very existence of vortex lattice melting, remains an open question.

In this superconducting films the interaction energy of two vortices located at the points $\mathbf{r}_i$ and $\mathbf{r}_j$ ($r_{ij}=|\mathbf{r}_i-\mathbf{r}_j|\gg\xi$) has the form[48]

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

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

$$\Phi(r_{ij})\approx\frac{\varphi_0^2}{4\pi^2 r_{ij}},\quad r_{ij}\gg\Lambda, \tag{28}$$

where $\Lambda(T)=2\lambda_B^2(T)/d$ is the effective penetration depth, d is the film thickness, λ_B is the bulk penetration depth, $\varphi_0=hc/2e$ is the flux quantum, $H_0(x)$ is the Struve function, and $Y_0(x)$ is a Neumann function.

The potential (28) is long-range (it is even "softer" than the Coulomb potential $1/r$). One might therefore expect, in accordance with the above discussion of two-dimensional melting, that a vortex lattice will melt by means of two continuous transitions.

The mean density $\langle n\rangle$ of the vortices in the system is related to the induction by the equation $B=\varphi_0\langle n\rangle$. In the case of a thin film, the demagnetization factor $N\to 1$ as $d/R\to 0$, where R is the characteristic dimension of the system, i.e., in the limit $d/R\to 0$ the vortex density has the form

$$\langle n\rangle=H/\varphi, \tag{29}$$

where H is the external magnetic field. With the help of Eq. (29), the melting curve of the vortex lattice can be constructed in the coordinates (T,H).

Note that the region of applicability of the vortex lattice melting theory using the potential (28) is bounded by the case of not-too-large fields, whose magnitude is determined by the condition $\xi(T)\ll a_0\propto\langle n\rangle^{-1/2}=(\varphi/H)^{1/2}$.

In order to construct the melting curve of a vortex lattice using the potential (28), we use an approximation analogous to Eqs. (24) and (25):

$$c^{(2)}(r;\langle n\rangle)=-\beta\Phi(r)\qquad\text{for } r\geqslant d_{\text{eff}}, \tag{30}$$

$$c^{(2)}(r;\langle n\rangle)=\bar{c}(r;\langle n\rangle)+(-\bar{c}(d_{\text{eff}};\langle n\rangle)-\beta\Phi(d_{\text{eff}}))\qquad\text{for } r<d_{\text{eff}} \tag{31}$$

d_{eff} is determined with the help of the effective liquid approximation. We take the short-range part of the direct correlation function $\bar{c}(r;\langle n\rangle)$ in the simple "rectangular" form:

$$c^{(2)}(r;\langle n\rangle)=-\beta\Phi(d_{\text{eff}})\qquad\text{for}\quad r\leqslant d_{\text{eff}}$$

(as has already been discussed for the case of a two-dimensional electron crystal, this result depends only slightly on the exact form of the short-range part).

By virtue of the long-range character of the interaction, the coupling constant of the dislocations is given by Eq. (11).

On the basis of the formulas we have obtained we have calculated the melting of a vortex lattice for the specific case of a niobium film of thickness 20 Å, which was investigated in detail experimentally in Ref. 49, from which we have taken the necessary parameters: $\xi(t)=\xi(0)/\sqrt{1-t}$, $\lambda_B(t)=\lambda(0)/\sqrt{1-t}$, $t=T/T_c$, $T_c\cong 3.66\text{K}$, $\xi(0)\cong 104\,\text{Å}$, $\lambda(0)\cong 1600\,\text{Å}$, and $dH_{c2}/dT=7$ kG/deg. Unfortunately, at the present time reliable estimates of the energy of the dislocation nucleus E_c in a vortex lattice in a superconductor are absent, so that in analogy with the case of a two-dimensional electron crystal we have assumed that $E_c=\bar{C}\mu a_0^2/4\pi$ and $\bar{C}=4.0$. Similarly, in the calculation of the curve of the transition from the hexatic phase to the isotropic liquid we used the approximation $E_d=\bar{c}\pi K_A(T)/72$, $\bar{c}\approx 3.0$.

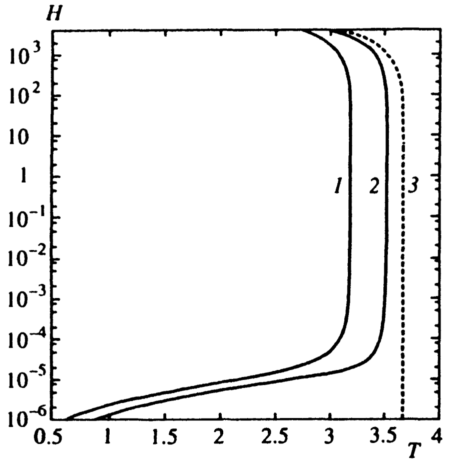

FIG. 1. Phase diagram of a system of vortices in a thin ($d=20$ Å) niobium film. Curve *1* is the melting line of the vortex lattice, curve *2* is the transition from the hexatic phase to the isotropic liquid, and curve *3* is the second critical field H_{c2}.

Figure 1 displays melting curves for a vortex lattice (curve 1), the hexatic phase–isotropic liquid transition (curve 2), and also the temperature dependence of the second critical field H_{c2} (curve 3). Note that the second critical field corresponds to the transition from the superconducting to the normal state in the mean field approximation. In reality, the transition coincides with the melting curve of the vortex lattice, and in the region between the melting curve and the second critical field H_{c2} there exists a local tendency for electrons to pair, but the superconducting order parameter field fluctuates strongly. In this state the system can be described in terms of mobile vortices—of the hexatic phase and the isotropic vortex liquid. The presence of mobile vortices, as is well known, leads to energy dissipation and the appearance of electrical resistance. Above H_{c2}, in the normal phase, the tendency toward local electron pairing disappears.

Figure 2 shows the same curves as in Fig. 1, but for the case $d=100$ Å with all the other parameters unchanged. As could be expected, since an increase in the film thickness substantially suppresses fluctuations of the superconducting order parameter, the melting line and the line of the transition from the hexatic phase to the isotropic liquid shift toward higher temperatures, and the existence region of the hexatic phase narrows. Our treatment of the melting of a vortex lattice is based on the assumption that vortices of only one sign exist with magnetic moments aligned with the field, whose density n_+ is given by expression (29). In thin superconducting films for $T>0$, thanks to thermal fluctuations, vortices of opposite sign n_- always exist (Refs. 51, 52); however, in the case of small fields we have $n_- \ll n_+$ (Refs. 51, 52), so that allowing for vortices of opposite sign should not qualitatively change the form of the melting curve. In addition, the case of intermediate fields requires additional consideration. Note also that in the case of small fields the jump in the resistance when the vortex lattice melts should be very small by virtue of the low vortex density and in reality the transition from the superconducting state to the normal state is a Kosterlitz–Thouless transition.[51,52]

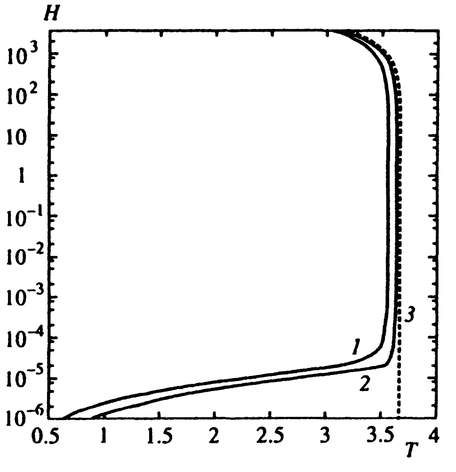

FIG. 2. Same as Fig. 1, but for a film of thickness $d=100$ Å .

Finally, note that we have not taken pinning into account, which is unavoidable in two-dimensional superconductors. The presence of frozen disorder can substantially change the character of the melting[32]; however, a consideration of this question lies outside the scope of the present paper.

6. CONCLUSION

Within the framework of the proposed theory, in systems with a long-range interaction such as a classical two-dimensional system of electrons or a system of vortices in a two-dimensional superconductor, the appearance of free dislocations causing the shear modulus to vanish and melting to take place before the mean-field thermodynamic instability $\Delta F=0$ is reached [see Eq. (4)]. In such cases the melting temperature T_m is lower than the temperature T_i of the instability of the hexatic phase with respect to formation of free disclinations, i.e., melting of a two-dimensional system with a long-range interaction proceeds via two continuous transitions. At the same time, in a system of hard disks the hexatic phase is unstable at all densities according to the physical picture described in the Introduction, and the system melts by way of a first-order transition coincident with the thermodynamic instability point. The results obtained for a system of 2D-electrons and a system of hard disks are in good agreement with the results of experiments, and also with computer simulations. In our opinion, this agreement could be improved by finding a more accurate form of the direct correlation function in the case of long-range potentials, and also by accounting for other terms besides $m=\pm 6$ in the expansion (13). However, we feel that the use of more accurate approximations should not alter the qualitative results obtained in this paper.

ACKNOWLEDGMENTS

This work was supported by the International Scientific Fund (Grant No. MUN000) and the Russian Fund for Fundamental Research (Grant No. 94-02-03415-a).

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Translated by Paul F. Schippnick