Transition to the superfluid state of a step on a free surface of a quantum crystal

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A study is reported of the zero-temperature phase diagram of a single step on the boundary separating a quantum crystal from vacuum. It is shown that an increase in the ratio of the amplitude of jumps of atoms along the step to the energy of a kink induces a phase transition of the step to the superfluid state. In this case the superfluidity does not imply phase coherence: the spatial correlations of the phase decay exponentially, exactly as in the normal state. At finite temperatures this zero-temperature superfluidity is destroyed, but in a wide range of parameters the linear friction coefficient (which depends on temperature in accordance with a power law) is exponentially small.

1. INTRODUCTION

Single steps on the free surface of a quantum crystal considered in the solid-on-solid (SOS) approximation can be described by the following Hamiltonian

$$H=\sum_j\left[\frac{J}{2}(\hat{n}_j-\hat{n}_{j-1})^2-Y\cos(\varphi_j-\varphi_{j-1})\right], \qquad (1)$$

where $\hat{n}_j\equiv -i\partial/\partial\varphi_j$ is the distance of this step from some fixed position, expressed in terms of the lattice constants (Fig. 1). The first term in Eq. (1) is the energy of the kinks on the step and the second represents quantum-tunneling jumps of atoms from the step (when n_j increases by unity and n_{j-1} decreases by unity and vice versa[1,2]) which occur with an amplitude $Y/2$ independent of n. The phase variables φ_j associated with n_j determine the local fluxes of the mass q along the step: $q_j=Y\sin(\varphi_j-\varphi_{j-1})$.

The Hamiltonian of Eq. (1) has two independent symmetry groups, one of which is discrete and the other continuous. They represent a simultaneous shift of all the values of n ($n_j\Rightarrow n_j+\Delta n$, where Δn is an integer), and simultaneous rotation of all the phases φ_j associated with conservation of the number of atoms. Consequently, two phase transitions can occur in the adopted model: from an atomically rough to an atomically smooth state and from the normal to the superfluid state. The atomically smooth state is distinguished from the rough state by the finite amplitude of the fluctuations of n: $\langle(\delta n)^2\rangle=\langle(n-\langle n\rangle)^2\rangle<\infty$ (which in the one-dimensional case may be attributed to the finite free energy of a kink[3]) and the superfluid state is understood in the usual way to mean that nondissipative mass transfer is possible (at least in the linear approximation). In the two-dimensional analog of the model of Eq. (1), which is used to describe the basal plane of a free surface of a quantum crystal, these two transitions may occur during cooling in a different order, which depends on the ratio of the parameters of the model.[2] In the one-dimensional model of Eq. (1) we would expect these phase transitions to occur at $T=0$ as a result of a change in the parameters.

Bradley and Doniach[4] used the model of Eq. (1) making an erroneous assumption that this can be used to describe a chain of series-connected tunnel junctions [in fact, an array of inverse capacitances with which the first term in Eq. (1) can be identified, should not contain negative components[5]]. In terms of a step the conclusion of these authors would imply that even at $T=0$ the step is in the normal (nonsuperfluid) state irrespective of the ratio of the parameters. We shall show that this is not true and that an increase of the parameter $\varkappa=Y/J$ in the model of Eq. (1) results in a transition from the normal to the superfluid state, whereas a transition to the atomically rough state does not occur when $\varkappa$ is varied. For comparison, we recall that the step on a quantum interface, which permits exchange of matter between the phases [when the Hamiltonian differs from Eq. (1) by the replacement of $\cos(\varphi_j-\varphi_{j-1})$ with $\cos\varphi_j$], undergoes a transition to the atomically rough state when $\varkappa$ increases in (Ref. 3).

It should be stressed that the use of the SOS approximation for the description of such a step implies that the free surface of a crystal (with a step on it) is in the atomically smooth superfluid state. The spectrum of excited states is then separated from the ground state by a gap[2] so that at zero or near-zero temperatures we can ignore any other fluctuations of the surface, apart from changes in the configuration of the step.

2. TRANSITION OF A STEP TO THE SUPERFLUID STATE

Elimination of n_j allows us to go over from the Hamiltonian (1) to the Lagrangian

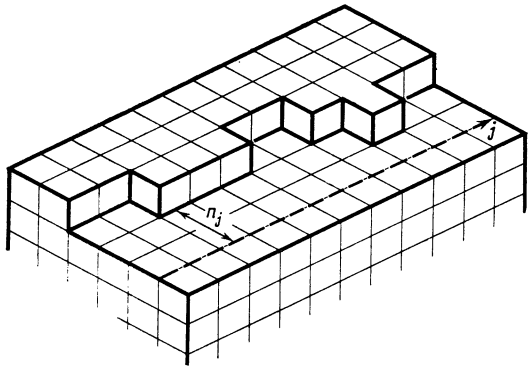

FIG. 1. Schematic representation of a step on the basal plane of a crystal with the simple cubic lattice. The SOS approximation is used and it is assumed that the step configuration can be described by specifying variables n_j which are integers and which represent the distances of various segments of the step from a certain straight line.

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$$L=\frac{U}{2}\Big(\sum_j \frac{\partial\varphi_j}{\partial\tau}\Big)^2-\sum_{j,l}\frac{\hbar^2}{4J}|j-l|\frac{\partial\varphi_j}{\partial\tau}\frac{\partial\varphi_l}{\partial\tau}$$

$$-\sum_j Y\cos(\varphi_j-\varphi_{j-1}),\quad U\to\infty, \tag{2}$$

which is written in the Euclidean form. The first two terms in Eq. (2) represent a positive definite quadratic form. In the semiclassical approximation ($Y\gg J$) the dominant role in the functional integral, which specifies the zero-temperature partition function of the model of Eq. (2), is played by instantons representing extremal paths of the Euclidean action

$$S=\int d\tau L\{\varphi\},$$

on which one or the other of the variables $\theta_j\equiv\varphi_j-\varphi_{j-1}$ overcomes the maximum of the period potential. In going around a saddle point along a distant closed path in two-dimensional space–time, we find that the circulation φ is $\pm 2\pi$ (Ref. 4) and the sign of the circulation can be regarded as the sign of the topological charge of an instanton.

In the model of Eq. (2) the effect of a single instanton is dispersed and it is finite only for a combination of instantons with zero net charge. For example, in the case of a pair of instantons of opposite sign, we have

$$S_2\approx\begin{cases}\pi\hbar(Y/J)^{1/2}R, & R^2\gg\Omega|\tau|\\ 2\pi^{1/2}\hbar(Y/J)^{1/2}|\Omega\tau|^{1/2} & \Omega|\tau|\gg R^2,1\end{cases}\qquad \Omega^2\equiv YJ/\hbar^2, \tag{3}$$

where R and τ are their distances in space and in imaginary time, respectively. The pair interaction of Eq. (3) can be described by the Green's function

$$G_0(k,\omega)=\frac{4\pi^2\hbar}{(\hbar^2/Y)\omega^2+J[2(1-\cos k)]^2} \tag{4}$$

and if $Y/J\gg 1$, instantons of different signs can form small pairs. Bradley and Doniach[4] assumed that since the pair interaction is stronger than logarithmic, dissociation of instanton pairs is altogether impossible.

A more consistent approach would require allowance for renormalization of the interaction of instantons by neutral pairs the concentration of which is finite for any ratio of the parameters. The correction to the Green's function $G_0^{-1}(k,\omega)$ of the principal (first) order in respect of the concentration of neutral pairs is[6]

$$\Sigma_1(k,\omega)=2z^2\sum_R\int d\tau[1-\cos(kR-\omega\tau)]$$

$$\times\exp\Big\{-\iint\frac{dk'\,d\omega'}{(2\pi)^2}[1-\cos(k'R-\omega'\tau)]G_0(k',\omega')\Big\}, \tag{5}$$

where z is the chemical activity of a single instanton, which in the case of low values of k and ω is

$$\Sigma_1(k,\omega)\approx\mu\omega^2+uk^2. \tag{6}$$

The first term in Eq. (6) represents only a slight quantitative renormalization of Y, given by

$$Y\to Y_R\equiv(Y^{-1}+4\pi^2\mu/\hbar)^{-1},$$

whereas the second alters the nature of the interaction of instantons at large distances so that the interaction becomes logarithmic:

$$S\approx K\ln(R^2+\Omega^2\tau^2)+C,\quad K=\pi(\hbar Y_R/u)^{1/2},\quad R^2+\Omega^2\tau^2\gg J/u.$$

Such a renormalization of the interaction of instantons is analogous to the renormalization of the interaction of disclinations by free dislocations in a two-dimensional smectic.[7]

If $\varkappa\gg 1$ the value of u is exponentially small in $\varkappa^{1/2}$ and the logarithmic interaction of instantons is sufficiently strong to ensure that they are still bound to form neutral pairs. This remains valid also if the Green's function $G_0(k,\omega)$ of Eq. (5) is replaced self-consistently by

$$G(k,\omega)=[G_0^{-1}(k,\omega)+\Sigma_1\{G\}]^{-1}, \tag{7}$$

which simply reduces K somewhat. If we include Σ_1, a pole of $G(k,\omega)$ corresponds to a linear spectrum of long-wavelength excitations which is typical of the superfluid state.

Reduction of $\varkappa$ reduces also K and when $K_{\min}=2$ is reached, instanton pairs dissociate (compare with Ref. 3), which corresponds to a transition of the investigated step from the superfluid to the normal state. At lower values of $\varkappa$, Eq. (7) no longer has a self-consistent solution and the long-range interaction of instantons is screened. The critical behavior in the vicinity of a phase transition point should then remain the same as in the usual Berezinskiĭ–Kosterlitz–Thoules transition because the origin of the logarithmic interaction of instantons over large distances is of no importance.

Additional evidence that an increase in $\varkappa$ induces a phase transition of the investigated step is provided if we note that for $Y\ll J$ the excited states of the step are separated from the ground state by a gap of width $2(J-Y)+O(Y^2/J)$, whereas in the opposite limiting case there is no gap in the spectrum.

The superfluidity is destroyed at finite temperatures. According to Ref. 3, the appearance of dissipation in one-dimensional models similar to that described by Eq. (2) considered in the semiclassical approximation may be associated with a nonzero probability of phase slip, i.e., the probability of incoherent tunneling of any of the variables $\theta_j=\varphi_j-\varphi_{j-1}$ to a neighboring minimum of the periodic potential. In the case of the logarithmic interaction of zero-temperature instantons the probability of quantum-fluctuation phase slip vanishes at low temperatures in accordance with a power law,[3] which in the problem under consideration implies a power-law temperature dependence of the linear friction coefficient γ: $\gamma\propto(T/\hbar\Omega)^{2K-2}$. Therefore, for the parameters corresponding at $T=0$ to the superfluid state of the step, which is not too close to the transition point the dissipation associated with mass transfer is exponentially small in terms of K if $K\gg 1$. On the other hand, as demonstrated earlier, if $\varkappa\gg 1$ the value of K is exponentially large in $\varkappa$, so that in this case γ is characterized by a double exponential smallness. If $T=0$ the friction coefficient γ vanishes, which demonstration of the superfluid properties of the state of the step.

3. ABSENCE OF PHASE COHERENCE IN THE SUPERFLUID STATE

Our analysis shows that if we allow for renormalizations due to a low concentration of bound instanton pairs, the asymptotic law of interaction of instantons in the model of Eq. (2) is logarithmic, i.e., it is exactly the same as in the

model with a somewhat different kinetic energy

$$L=\sum_j\left[\frac{m}{2}\left(\frac{\partial\varphi_j}{\partial\tau}\right)^2-V\cos(\varphi_j-\varphi_{j-1})\right], \tag{8}$$

investigated in Refs. 3 and 4 as a model suitable for the description of a regular chain of tunnel junctions coupled by capacitances on a conducting substrate. It is worth recalling that in the model of Eq. (8) the superconducting phase differs from the normal phase not only because the linear friction coefficient vanishes,[3] but also because the nature of the behavior of the one-time correlation function is different:

$$F(R)=\langle\exp\{i[\varphi_{j+R}(t)-\varphi_j(t)]\}\rangle. \tag{9}$$

For the normal phase the function $F(R)$ decreases exponentially, whereas in the superconducting state it obeys a power law[4] (quasilong-range order). On the other hand, in the model (2) characterized by similar thermodynamic properties the correlation function of Eq. (9) decays exponentially in the normal and superfluid phases. This can be demonstrated by representing $F(R)$ in the form

$$F(R)\approx\exp\left[-\iint\frac{dk\,d\omega}{(2\pi)^2}(1-\cos kR)\,g(k,\omega)\right],$$
$$g(k,\omega)=\int d\tau\sum_R\langle\varphi_{j+R}(\tau_0+\tau)\varphi_j(\tau_0)\rangle\exp(-ikR+i\omega\tau), \tag{10}$$

which follows from the assumption that fluctuations are Gaussian. In general, such a representation is valid only for the superfluid phase in which there are no free excitations with nonzero topological charges.

In the semiclassical approximation the correlation function can be calculated as a sum of two terms,[4,6] one of which

$$g_0(k,\omega)=\hbar\Big/\left\{2(1-\cos k)\,Y+\frac{\hbar^2}{J}\frac{\omega^2}{2(1-\cos k)}\right\} \tag{11}$$

is related to small oscillations of φ and the other $[g_{in}(k,\omega)]$ is associated with instanton pairs. If we assume that in the case of a single instanton pair at a large distance from it we have

$$\varphi_j(\tau)\approx\Phi(j-R_1,\tau-\tau_1)-\Phi(j-R_2,\tau-\tau_2)$$
$$\approx\Delta\tau(\partial_\tau\Phi)+\Delta R(\partial_j\Phi),$$

where $\Phi(j,\tau)$ is the explicit form of an instanton path, whereas $\Delta R=R_2-R_1$ and $\Delta\tau=\tau_2-\tau_1$ are the relative separations—in space and in imaginary time—of instantons forming a pair, averaging over the whole volume ignoring correlations of different pairs gives

$$g_{in}(k,\omega)=[\partial_\tau\Phi]_{k\omega}[\partial_\tau\Phi]_{k\omega}^*\langle(\Delta\tau)^2\rangle c$$
$$+[\partial_j\Phi]_{k\omega}[\partial_j\Phi]_{k\omega}^*\langle(\Delta R)^2\rangle c. \tag{12}$$

Here c is the concentration of instanton pairs and the square brackets with the indices k and ω represent the Fourier transforms of the derivatives Φ ($\partial_j\Phi$ is naturally understood to be the lattice derivative). If we use Eq. (10), it is convenient to express $g_{in}(k,\omega)$ in terms of the derivatives of $\Phi(j,\tau)$ because the function itself is multivalued.

The divergence of the exponential function in Eq. (10) is governed by the behavior of $g(k,\omega)$ at low values of k and, consequently, it is determined by the asymptotic nature of an instanton path far from a saddle point. According to Ref. 8, this asymptotic form can be found if we replace the cosine potential with a harmonic one, so that in the model of Eq. (2) when $k,\omega\to0$ we have

$$[\partial_\tau\Phi]_{k\omega}\approx\pm2\pi\Omega^2\frac{(ik)^3}{\omega^2+\Omega^2k^4},$$
$$[\partial_j\Phi]_{k\omega}\approx\mp2\pi\frac{+i\omega}{\omega^2+\Omega^2k^4}. \tag{13}$$

It should be noted that

$$+i\omega[\partial_j\Phi]_{k\omega}+ik[\partial_\tau\Phi]_{k\omega}$$

is then equal to $\pm2\pi$ and not to zero (in contrast to a single-valued function), which reflects the appearance of a branching point when $\Phi(j,\tau)$ goes to the continuous limit.

Substitution of Eq. (13) into Eq. (12) demonstrates that the first term in Eq. (12), like that in Eq. (11), does not result in unlimited reduction in $F(R)$ for $R\to\infty$, whereas the second term in Eq. (12) gives rise to an exponential decay of $F(R)$. The correlation radius is then governed by the concentration of different-site instanton pairs and for $\varkappa\gg1$ it is exponentially large in $\varkappa^{1/2}$.

It therefore follows that the phase coherence (understood as the existence of long-range quasiorder represented by a decay of the correlation function in accordance with a power law) is absent not only in the normal but also in the superfluid state. Starting from the exponential nature of the decay[1)] of $F(R)$ at high values of $\varkappa$, Bradley and Doniach reached the incorrect conclusion that the model of Eq. (2) predicts that there should be no phase transition to the superfluid state.[4]

In reality the superfluidity (superconductivity) of one-dimensional quantum systems, by which is understood the vanishing of the linear friction coefficient, is far from identical with the power-law decay of the correlation function of Eq. (9). Attention to this point was first drawn by Matthew Fisher, who considered a chain of series-connected noninteracting tunnel junctions with linear ohmic dissipation, the Lagrangian of which can be represented as a sum of independent Lagrangians of the individual contacts.[9] In the case of high values of the effective viscosity such a chain as a whole is in the superfluid state (and phase slip is completely suppressed), although the correlation of the phase along it decays strictly in accordance with the exponential law. It follows from the above discussion that this applies also to the model of Eq. (2), which does not allow such splitting into noninteracting degrees of freedom.

4. CONCLUSIONS

It therefore follows from the model of Eq. (1) that an increase in the ratio of the amplitude of quantum-tunnel jumps of atoms along a step to the energy of an elementary kink causes a step on a free surface of a quantum crystal to undergo a phase transition to the superfluid state. Although in this state the one-time correlation function of Eq. (9) falls exponentially, exactly as in the nonsuperfluid state (so that we cannot speak of the phase coherence), the linear friction coefficient vanishes in the superfluid state. At finite tem-

peratures this zero-temperature superfluidity is destroyed, but over a wide range of parameters the friction coefficient, which exhibits a power-law temperature dependence, is exponentially small. We can expect similar properties to be exhibited also by distant steps on weakly inclined (vicinal) faces.

The possibility of nondissipative (or quasinondissipative) mass transfer on the free surface of a quantum crystal has become important because of the experimental detection of superplasticity of para-hydrogen single crystals,[10] which can be explained by surface mass transfer.[11] It would therefore be of interest to investigate systematically the dynamic properties of the surfaces of para-hydrogen single crystals at low temperatures.

The transition to the superfluid state investigated by us is unrelated to the transition to a rough surface. In the semiclassical approximation the amplitude of quantum fluctuations of the position of the step $\langle(\delta n)^2\rangle^{1/2}$ is finite in the model of Eq. (1) even if we ignore instantons. Since the presence of instantons (in free or bound form) simply reduces $\langle(\delta n)^2\rangle$ (Ref. 8), such a step is in an atomically smooth state at $T=0$ irrespective of the ratio of the parameters. It therefore follows that the normal and superfluid states are both atomically smooth at zero temperature. At any other low temperature the step goes over to an atomically rough state because of the appearance of thermally activated kinks.

Kampf and Schön[12] discovered a zero-temperature phase transition in the model (1) by a variational approximation. However, this method is unreliable (in particular, it predicts stability of the superfluid state also for $T>0$ and yields results known to be incorrect in the case of a zero-dimensional system), so that the results obtained by them cannot be regarded as other than accidental.

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[1)] It should be pointed out that the treatment in Ref. 4 allows only for one-site instanton pairs, which—according to our calculations—should not result in unlimited decay of $F(R)$. However, the authors of Ref. 4 used in their calculations the expression for $\Phi(j,\tau)$ which on the $\tau=0$ axis is a physically meaningless cut. It follows from the results that these two mistakes to some extent cancel one another, so that the dependence $F(R)$ remains exponential, as expected.

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