

Phase Transitions on Quantum Crystal Interfaces

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The quantum solid-on-solid (SOS) model for the free surface of a crystal is studied at zero and finite temperatures. In addition to the usual roughening transition, this model also exhibits a superfluid transition. The phase diagram is constructed. We also formulate and study a quantum SOS model for the solid-liquid interface, which takes into account the motion and the compressibility of the liquid and solid. The existence of a phase transition at zero temperature is shown. The phases differ in the form of the excitation spectrum. In both interface models the interface at zero temperature is smooth. The quantum effects only slightly reduce the temperature of the roughening transition in comparison to the classical value.

1. INTRODUCTION

Following the pioneering work by Andreev and Parshin¹ and the discovery of freezing-melting waves on the solid-liquid ⁴He interface,² quantum phenomena on crystal faces have become the subject of intensive theoretical and experimental studies.

The main assumption made by Andreev and Parshin,¹ of the possibility of quantum roughening at zero temperature for a great enough interface hopping of atoms, was criticized by Fisher and Weeks,³ who noted the finite amplitude of the zero oscillations of a crystal surface (in contrast to the case of thermal fluctuations) and the consequent sensitivity of the position of the interface to the atomic crystal structure. Accordingly, they stated that any face must be smooth at absolute zero.

In a previous paper⁴ we considered a simple model of the quantum interface, corresponding to atomic transitions without the excitation of the liquid, i.e., hopping to and from the Bose condensate, with the superliquid being in the ground state. In this model there is no phase transition with respect to a quantum parameter at zero temperature and any face is smooth, as was conjectured by Fisher and Weeks.³

In this paper we investigate phase transitions in a model where atoms of the crystal hop only along its surface without changing their number. Such a model describes faces of a quantum crystal existing at zero pressure and was introduced by Fradkin,⁵ who has shown that at zero temperature the crystal faces are smooth.

In addition, we construct a model for the solid-liquid ⁴He interface with excitation of the superfluid and describe the phase transitions in such a case.

The previous result concerning the smoothness of the crystal faces³⁻⁵ is valid here, but in these models other kinds of phase transitions also appear. Some results of this paper have been published previously.⁶

2. VACUUM-QUANTUM CRYSTAL INTERFACE

The quantum solid-on-solid (SOS) model of the free surface of a crystal introduced by Fradkin⁵ has the Hamiltonian

$$H = \sum_{(jl)} \left[\frac{J}{2} (n_j - n_l)^2 - \frac{\mu}{2} (a_j^+ a_l^- + a_j^- a_l^+) \right] \quad (1)$$

The integer variables n_j are described on the sites of a two-dimensional lattice and represent the height of the crystal surface with respect to a certain level. The summation in (1) is performed over pairs of nearest neighbors. The first term in the square brackets is the potential energy related to the configuration of the surface. The operators a_j^+ and a_j^- change n_j into $n_j + 1$ and $n_j - 1$, respectively. Thus the product $a_j^+ a_l^-$ describes the hopping of an atom from site l to site j . For simplicity it is assumed in (1) that atoms hop only to nearest neighboring sites and that the hopping probability μ does not depend on the configuration $\{n_j\}$.

Introducing variables φ_j that are Hamiltonian conjugate to n_j , we can rewrite (1) as

$$H = \sum_{(jl)} \left[\frac{J}{2} (n_j - n_l)^2 - \mu \cos(\varphi_j - \varphi_l) \right]; \quad n_j = -i \frac{\partial}{\partial \varphi_j} \quad (2)$$

Fradkin⁵ did not deal directly with (2), but introduced instead a sine-Gordon Hamiltonian with continuous variables n_j that has the same symmetry as (2). He showed that for such a Hamiltonian at zero temperature the crystal surface is smooth for any finite ratio μ/J . He also showed that the temperature of the roughening transition T_R does not depend on the magnitude of the quantum parameter μ .

We stress that the Hamiltonian (2) has two independent groups of symmetries: (1) the discrete group of a simultaneous shift of all n_j and (2)

the continuous group of a simultaneous rotation of all φ_j . Accordingly, there must be two different phase transitions. The transition from a rough to a smooth phase of the surface leads to the spontaneous breaking of first symmetry. The existence of the other phase transition becomes evident in the case $J = 0$, when the Hamiltonian (2) reduces to the Hamiltonian of the classical XY model, which is well known to have a phase transition (at finite temperature) connected with the dissociation of vortex pairs.⁷⁻¹⁰

We intend to verify that this second transition also exists in the case of nonzero J . In order to do this, we begin with the investigation of the model given by (2) at zero temperature. The method we use enables us also to draw conclusions about the smoothness of the surface directly for the Hamiltonian (2).

For $\mu = 0$ the energy (2) of the ground state is also zero. The lowest excited states have the energy $Jz/2$ (z is the number of nearest neighbors). These states are highly degenerate (twice the number of lattice sites). In the case $\mu \ll J$ we can treat (2) with the help of perturbation theory. The first-order correction splits the excited level $Jz/2$ into a band with a width $z\mu$, but does not affect the energy of the ground state. Taking into account higher order corrections, we obtain a finite value of the excitation gap, which can be written as

$$\frac{1}{2}z(J - \mu) + O(\mu^2/J)$$

for sufficiently small μ/J .

In the case $\mu \gg J$ it is convenient to work with the functional integral representing the Feynman transition amplitude¹¹ for the Hamiltonian (2). This amplitude can be written as

$$Z = \lim_{\tau \rightarrow 0} \prod_{jt} \left[\sum_{m_j(t)=-\infty}^{\infty} \int_{-\infty}^{\infty} dn_j(t) \int_{-\pi}^{\pi} d\varphi_j(t) \right] \times \exp \left(-\sum_i \left\{ \frac{\tau}{\hbar} H(n, \varphi) - i \sum_j n_j(t) [\varphi_j(t+\tau) - \varphi_j(t) - 2\pi m_j(t)] \right\} \right) \quad (3)$$

where we have performed the transition to imaginary discrete time and have replaced summations over $n_j(t)$ by integrations, simultaneously adding delta-functional multipliers in the form of sums over $m_j(t)$.

For $\mu \gg J$ one can evaluate this functional integral by calculating different terms of the sum $m_j(t)$ with the help of the saddle point method (this procedure is explained more thoroughly in Ref. 4, where we treated a simpler quantum SOS model). The extremum of the action in the exponent in Eq. (3) corresponds to the trajectory satisfying the classical equations of

motion for φ and n :

$$\begin{aligned}
 i\frac{\partial\varphi_j}{\partial t} &= -\frac{1}{\hbar}\frac{\partial H}{\partial h_j} + 2\pi i\tilde{m}_j = \frac{J}{\hbar}\partial_\gamma^2 n_j + 2\pi i\tilde{m}_j(t) \\
 \tilde{m}_j(t) &= \sum_{t_i} m(t_i)\delta(t-t_i) \\
 i\frac{\partial n_j}{\partial t} &= \frac{1}{\hbar}\frac{\partial H}{\partial\varphi_j} = \frac{\mu}{\hbar}\sum_\gamma [\sin(\varphi_{j+l_\gamma} - \varphi_j) - \sin(\varphi_j - \varphi_{j-l_\gamma})] \\
 &\equiv \frac{\mu}{\hbar}\partial_\gamma \sin \partial_\gamma \varphi_j
 \end{aligned} \tag{4}$$

where ∂_γ denotes the lattice gradient.

Consider the solution of Eqs. (4) corresponding to $m_j(t)$ nonzero at only one site (say $j=0$) at one single moment of time (say $t=0$). After excluding n from Eqs. (4), one obtains an equation for φ :

$$\frac{\partial^2\varphi_j}{\partial t^2} + \frac{\mu J}{\hbar^2}\partial_\beta^2\partial_\gamma \sin \partial_\gamma \varphi_j = 2\pi\frac{\partial}{\partial t}\tilde{m}_j = 2\pi m_0\frac{\partial}{\partial t}\delta(t) \tag{5}$$

The linearized version of Eq. (5) under Fourier transformation (in space-time) becomes a linear algebraic equation. Its solution for small k , ω is

$$\varphi_0(k, \omega) = \frac{2\pi i\omega}{\hbar^{-2}J\mu(ak)^4 + \omega^2} \tag{6}$$

where a is the lattice spacing.

The left-hand side of Eq. (5) has the form of the divergence of some vector constructed from the derivatives of φ (more precisely, their finite difference counterpart). If we multiply (5) by t , we obtain an equation whose left-hand side also has the form of a divergence [of a vector with components $(t\partial\varphi/\partial t - \varphi, \partial_\beta\partial_\gamma \sin \partial_\gamma \varphi)$]. This property of Eq. (5) enables us to find its solution at large distances (in space-time) where the continuous approximation is valid. The singularity on the right-hand side determines this solution uniquely. Since large distances correspond to small momenta and frequencies, we have

$$\varphi(k, \omega) = \varphi_0(k, \omega) + \text{higher order terms in } k \text{ and } \omega$$

Combining this result with Eqs. (4), one can find the Fourier transform of $n_j(t)$, which we shall denote as $2\pi iG_0(k, \omega)$. For small k

$$G_0(k, \omega) = \frac{\hbar}{Jk^2 + (1/\mu)(\hbar\omega/a^2k)^2} \tag{7}$$

$G_0(k, \omega)$ coincides with the “bare” (for continuous n) Green’s function (correlator $\langle n_{k\omega} n_{-k, -\omega} \rangle$). It can be obtained from (2) if one neglects the discreteness of n and the periodicity in φ , i.e., substitutes $-1 + \frac{1}{2}(\varphi_j - \varphi_l)^2$ for $-\cos(\varphi_j - \varphi_l)$. We see that the bare excitation spectrum for long wavelengths corresponds to $\omega \sim k^2$.

The action on the extremal path considered here (in field theory it is called an “instanton”) is large [proportional to $(\mu/J)^{1/2}$] but finite. The convergence of the corresponding integral is connected with the form of $G_0(k, \omega)$ for small k and ω , which is known exactly. Thus the terms with $m_j(t) \neq 0$ are relatively small. For a typical term in Z [Eq. (3)] the nonzero $m_j(t)$ (which can be thought of as charges of “instantons”) are far from one another (in space-time).

For $\mu \gg J$ Eq. (3) can be rewritten as the partition function of the instanton gas with the interaction $g_0(R, t)$,

$$Z \propto \sum_{m_j(t)} \exp \left[-\frac{1}{2} \sum_{jj', tt'} 4\pi^2 g_0(R_j - R_{j'}, t - t') m_j(t) m_{j'}(t') \right] \quad (8)$$

where $g_0(R, t)$ results from the Fourier transformation of $G_0(k, \omega)$, and $g_0(0, 0) \propto (\mu/J)^{1/2}$.

The concentration of instantons in space-time is low:

$$C \sim (\mu^3 J)^{1/4} \exp[-c_1(\mu/J)^{1/2}] \quad (9)$$

where the dimensionless coefficient c_1 depends on the exact form of G_0 for large k and ω . The quantity $c_1(\mu/J)^{1/2}$ is the action on the extremal “one instanton” path, which is calculated by means of G_0 . The calculation of the preexponential factor in Eq. (9) requires Gaussian integration in the vicinity of the extremal path (for details see, e.g., Ref. 12).

Thus in the case of $\mu \gg J$ all the conditions for the validity of the self-consistent approximation (SCA) are fulfilled. The long-range interaction of charges is small for typical distances between them. The mutual screening of the charges affects the Green’s function. In the SCA this change corresponds to adding the constant self-energy, which is proportional to C :

$$G^{-1}(k, \omega) = G_0^{-1}(k, \omega) + (4\pi^2/\hbar)C \quad (10)$$

where C must be expressed in terms of G self-consistently. A more thorough treatment changes higher order terms in k and ω in Eq. (10), which are of minor significance.

It is clear from Eq. (10) that notwithstanding the finite concentration of instantons, the spectrum of excitations remains gapless. For small k its form becomes acoustic, $\omega = c_s k$ ($c_s^2 \propto C$).

Equation (10) is valid only for sufficiently large μ/J when the saddle point method can be used. We have established previously that in the

opposite limit of small μ/J the spectrum has a gap. Thus there is a phase transition at zero temperature. In addition to the change in the form of the spectrum this transition also effects the behavior of the correlation functions. If one considers the correlation function $\langle \cos [\varphi_j(t) - \varphi_i(t)] \rangle$ for $|r_j - r_i| \rightarrow \infty$ one can verify that for the low- (μ/J) phase it decays exponentially, while for the high- (μ/J) phase it has a finite limit. Thus the transition at zero temperature is of the same nature as the transition at zero J , when the model (2) coincides with the classical XY model. The surface of this phase transition in (J, μ, T) space connects a straight line in the (T, μ) plane with a straight line in the (J, μ) plane.

We stress that this transition has nothing to do with the roughening transition. Both phases are smooth at zero temperature. As we have shown previously⁴ for a wide class of models, including (2), the energy of a step on a crystal surface is determined by a gap in the correlation function for zero frequency and not by a gap in the excitation spectrum. Thus, for $G(k, \omega)$ defined by Eq. (10) the energy of a step is finite and the surface is smooth. The phase transition in the XY model is associated with the dissociation of vortex pairs.^{8,9} The vortices are nontrivial solutions of Eq. (4) for $m_j(t) = 0$. The existence of such solutions is due to the periodicity in φ (which enables us to consider the solutions with nonzero circulation) and due to the invariance of the Hamiltonian (2) with respect to the rotation of all φ_j .

In the case $J = 0$ only stationary vortices are permitted. The action corresponding to a single vortex is proportional to μ/T [at finite temperature T the time integration in the exponent of Eq. (3) is restricted to the interval $(0, \hbar/T)$] and diverges logarithmically with increasing size of the system. Only for pairs of vortices with opposite signs is the action finite. At sufficiently high temperature, vortex pairs dissociate and this causes the action of a single vortex to become finite due to screening.^{9,10}

For $T = 0$ this mechanism does not operate, but for $J \neq 0$ other factors make the creation of a free vortex possible. A vortex can move in imaginary time from site to site, and vortex pairs can be created and annihilated, thus forming vortex loops in space-time. There is also a finite density of instantons in the system. It is possible to show that the presence of instantons is sufficient to induce the formation of free vortices at $T = 0$.

Let us consider the interaction of an instanton and a vortex. Almost everywhere but near the center of the instanton and the vortex core the absolute value of $\partial_\gamma \varphi$ is small compared to unity. This enables us to substitute the first few terms of the Taylor expansion for $\cos(\varphi_j - \varphi_i)$. In the quadratic approximation, however, the interaction between the instanton and the vortex is absent and the action is the sum of separate contributions for the instanton and the vortex (solenoidal and potential fields of the velocity do

not interact). The interaction arises only in the higher terms of the Taylor expansion. The sign of the most important quartic term corresponds to the attraction of a vortex and an instanton of any charge. The magnitude of the interaction is given by

$$V = -\frac{\mu}{24} \int \frac{dt d^2r}{\hbar} \sum_{\gamma} \left(\frac{\partial \varphi_{\text{inst}}}{\partial r_{\gamma}} \right)^2 \left(\frac{\partial \varphi_{\text{vort}}}{\partial r_{\gamma}} \right)^2$$

in the continuous approximation, where φ_{inst} and φ_{vort} denote the field for the instanton and the vortex, respectively.

The main contribution to the integral comes from the center of the instanton, because $\partial_{\gamma} \varphi_{\text{inst}}$ falls off rapidly at a distance of several atomic lengths from it. For this reason $\partial_{\gamma}^2 \varphi_{\text{inst}}$ can be considered as a constant proportional to R^{-2} , where R is the distance between the instanton and the vortex. Performing the integration over $dt d^2r$, we see that

$$V \propto -\left(\frac{\mu}{J}\right)^{1/2} \frac{1}{R^2} \quad (11)$$

The action for a “bare” vortex of unit length in the time direction is positive and logarithmically divergent. It is clear from Eq. (11) that the total contribution from the vortex interaction with an instanton gas of finite concentration C also is logarithmically divergent. For large enough C this negative term can dominate and induce formation of free vortices. There are also other causes diminishing the vortex action (e.g., vortex loops in space-time).

As mentioned above, this phase transition has the same physical origin as the phase transition in the plane XY model and corresponds to the destruction of the surface superfluidity in this model. This superfluidity has the usual meaning: the possibility of nondissipative mass flow along the quantum crystal face at sufficiently small J .

3. THE STRUCTURE OF THE PHASE DIAGRAM

In order to have a phase diagram we must consider the case of finite J , μ , T . For finite temperatures, Eq. (7) for a “bare” Green’s function is also valid but with discrete frequencies $\omega_l = 2\pi lT$, where l is an integer. Accordingly, the interaction of the instantons changes and becomes

$$g(\mathbf{R}, t) = \frac{T}{2\pi J} \ln |\mathbf{R}| + T \sum_{l \neq 0} \int \frac{d^2k}{(2\pi)^2} \frac{1}{Jk^2 + (1/\mu)(\hbar\omega/a^2k)^2} e^{i(k\mathbf{R} - \omega_l t)} \quad (12)$$

The appropriate chemical potential of the instanton $g(0)$ is logarithmically divergent at small k and we have $g(0) \sim (T/2\pi J) \ln(L/R_0)$, where L

is the macroscopic length (the size of the interface) and $R_0 \sim \exp[\frac{1}{2}c_1(\mu/J)^{1/2}]$. Thus the quantum hopping affects only R_0 . According to a well-known entropy argument, the phase transition occurs at $2T/\pi J \approx 1$. It manifests itself in the appearance of “free” instantons.

It follows from the renormalization group analysis by Kosterlitz¹⁰ that at $T/J < \pi/2$ the face will be smooth for any R_0 . Hence the temperature of the phase transition T_R in this model decreases with increasing μ , but cannot be lower than $T_R^{\text{min}} = \pi J/2$. This phase transition is the usual roughening transition.^{13,14} The free energy of a step on the face [which is defined by the zero frequency correlator⁴ $G(\omega = 0, k)$] vanishes at the transition temperature.

Summarizing this result and the results of the previous section, we obtain the picture of the phase transitions shown in Fig. 1. The surface of the roughening transition (which is almost plane) connects the μ axis and the straight line $J/T = \text{const}$ on the plane $\mu = 0$ for the roughening transition of the classical discrete Gaussian model.¹⁴

In addition, there is a surface of the transition to the superfluid phase (on the crystal face) which connects the straight line $\mu/T = \text{const}$ on the plane $J = 0$ corresponding to the classical 2d XY model, and the straight line $\mu/J = \text{const}$ on the plane $T = 0$ corresponding to the vanishing of the gap in the elementary excitation spectrum. So we have four different phases: phase 1 corresponds to the rough superliquid phase, phase 2 to the rough normal phase, phase 3 to the smooth normal phase, and phase 4 to the smooth superfluid phase. The instantons are present only in the smooth phases (3 and 4), and the free vortices exist only in the normal (nonsuperfluid) phases (2 and 3). It is possible that the line where all four phases coexist splits into two triple lines.

Note that in the smooth superfluid phase 4 special “faceting” waves with acoustic spectrum $\omega = c_s k$ can be observed, analogous to freezing-melting waves. These “faceting” waves also correspond to quantum oscillations of the crystal faces, but in the absence of the melt, due only to quantum motion of atoms of the crystal near its free surface.

Actually, quantum effects are observed in ³He and ⁴He crystals only. These crystals exist only at nonzero pressures and the model considered

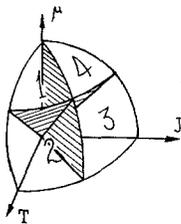


Fig. 1. Possible phase diagram for a quantum SOS model of a crystal-vacuum interface.

cannot be applied to them directly. It is possible that this model can be applied to hydrogen or crystals of other inert gases that exist at zero pressure.

We can speculate also that this model can be applied to the solid-normal liquid ^3He interface. This can be justified if one assumes that an atom cannot go from the solid to the liquid without strongly exciting the liquid. If we exclude the excited states of the liquid in the second order of perturbation theory, we obtain the effective Hamiltonian in the form of Eq. (2).

4. SOLID-SUPERFLUID INTERFACE

In the simplest quantum SOS model considered by us previously⁴ the motion of the liquid was not taken into account. Instead it was supposed that the atomic exchange between the solid and the liquid does not change the state of the latter. This assumption is justified only in the case of equal densities of the crystal ρ_C and of the liquid ρ_L .

Constructing a more realistic model for the quantum tunneling of an atom from the crystal to the liquid, we assume the appropriate term in the Hamiltonian in the form $\mu_j a_j^-$. The quantity μ_j is complex and since it is associated with the change of the total number of atoms in the liquid, its phase χ_j coincides with that of the Bose condensate of the superfluid (i.e., ^4He). The appropriate surface energy takes the form

$$H_S = \frac{J}{2} \sum_{\langle j,l \rangle} (n_j - n_l)^2 - A \sum_j \cos(\varphi_j - \chi_j) \quad (13)$$

Here χ_j is the value of the condensate phase χ on the face site j , and n_j denotes the position of the interface with respect to the undeformed solid (in lattice units); as previously, $n_j = -i \partial / \partial \varphi_j$. For simplicity the summation in the first term is restricted to the nearest neighbors, as in Section 1, and the real quantity A is assumed to be independent of the configuration $\{n_j\}$. Only the long-wave properties of the model are important and the exact form of the lattice cutoff for hydrodynamic quantities is of no significance.

In order to have a consistent quantum mechanical model we must define the action on the phase trajectories of the system. It is quite natural to take the total action as the sum of the three actions $S_L + S_C + S_S$ for the liquid, the crystal, and the interface, respectively.

The action of the superfluid is given by

$$S_L = - \int dt \int_{V_L} d^3r \left[\rho_L \frac{\hbar}{m} \frac{\partial \chi}{\partial t} + \rho_L \frac{\hbar^2}{2m^2} (\nabla \chi)^2 + E_L(\rho_L) \right] \quad (14)$$

where $E_L(\rho_L)$ is the internal energy density of the liquid and m is the atomic

mass, and the interaction is performed over the real volume of the liquid V_L restricted by the interface.

The form of the action for the crystal is taken from elasticity theory:

$$S_C = \int dt \int_{V_C} d^3r \left(p_C \frac{du}{dt} - \frac{p_C^2}{2\rho_C} - E_C \right) \quad (15)$$

where u is the displacement vector, E_C is the internal energy density, which depends on the deformation tensor u^{ik} , V_C is the real volume of the crystal, and p_C is the volume density of the momentum $p_C = \rho_C v_C$.

The interface part of the action is

$$S_S = - \int dt \left(\hbar \sum_j n_j \frac{\partial \varphi_j}{\partial t} + H_S \right) \quad (16)$$

where H_S is given by Eq. (13).

In Ref. 6 we have used in the surface energy the term $-A \cos(\varphi_j - \lambda \chi_j)$ with $\lambda \neq 1$ and a slightly different form of S_L . Both versions have the same equations of motion and are equivalent.

As in the previous sections, we investigate the model in the limit of an almost rough interface with small J and large A and in the opposite case of small A , when the interface must be close to a plane.

In the first case we can transform the partition function (or Feynman amplitude for the imaginary time; see Section 1) into the partition function of some instanton gas, using the saddle point method. The appropriate equations of motion, obtained by the variation of the action in terms of the independent variables χ , ρ_L , p_C , and u , have the usual form of hydrodynamic equations for the liquid and that of elasticity theory for the solid:

$$\frac{\partial}{\partial t} \rho_L + \text{div}(\rho_L v_L) = 0; \quad \frac{\hbar}{m} \frac{\partial \chi}{\partial t} + \frac{v_L^2}{2} + \mu_L = 0 \quad (17)$$

$$v_C = \frac{du}{dt}; \quad \rho_C \frac{d}{dt} v_C^i = \frac{\partial \sigma^{ik}}{\partial x^k} \quad (18)$$

where $v_L = (\hbar/m)(\nabla \chi)$ is the velocity of the liquid, $\mu_L = \partial F_L / \partial \rho_L$ is the chemical potential of the liquid, and σ^{ik} is the stress tensor of the solid.

The variation of the action in terms of the surface quantities φ , χ_s , u_s , and n (n is treated as continuous) gives, after some transformations, the boundary conditions

$$\hbar \partial n_j / \partial t = A \sin(\varphi_j - \chi_j) \quad (19)$$

$$\rho_L (v_L^v - w^v) = \rho_C (v_C^v - w^v) \quad (20)$$

$$p_L \delta^{iv} + v_L^i (v_L^v - w^v) \rho_L = -\sigma^{iv} + v_C^i (v_C^v - w^v) \rho_C \quad (21)$$

$$\mu_L + \frac{1}{2}(v_L - v_C)^2 - \mu_C(p_L) = \frac{1}{m} \left[\frac{\hbar^2}{A \cos(\varphi_j - \chi_j)} \frac{\partial^2 n_j}{\partial t^2} - J \Delta^L n_j \right] \quad (22)$$

where ν denotes the normal to the interface, w^ν is the velocity of the normal motion of the interface, p_L is the pressure of the liquid, Δ^L is the lattice Laplacian, and $\mu_C(p_L) = (E_C + p_L)/\rho_C$.

Equations (20) and (21) are mass and momentum conservation equations, respectively. Equation (22) is a generalisation of the Herring condition for the solid-liquid interface. This equation includes a specific interfacial inertial term, which was introduced phenomenologically by Puech and Castaing.¹⁵ The other term on the right-hand side of Eq. (22) is related to the curvature of the interface with respect to the undeformed crystal. Comparing Eq. (22) with its phenomenologically derived dissipative counterpart,¹⁶ one can verify that it is only this "reduced" curvature that must enter the equation. In what follows, for simplicity we neglect the compressibility of the solid and use the linearized equations of motion in the continuous limit with the lattice cutoff.

In this approximation we obtain from Eqs. (17) and (19)–(22) the bare Green's function for variable n :

$$G_0(k, \omega) = \frac{\hbar}{Jk^2 + [\hbar^2/Aa^2 + \rho_{\text{eff}}d^2(k^2 + \omega^2/c^2)^{-1/2}]\omega^2} \quad (23)$$

$$\rho_{\text{eff}} = \frac{(\rho_C - \rho_L)^2}{\rho_L}$$

where a is the lattice constant (in the plane of the face), d is the interplanar distance, and $c_L^2 = \partial p_L / \partial \rho_L$ is the squared sound velocity for the liquid, and we again are dealing with imaginary time. The poles of Eq. (23) define the bare spectrum of surface excitations (if the discreteness of n is neglected). This spectrum coincides with the phenomenologically derived spectrum of freezing-melting waves ($\omega \propto k^{3/2}$ for small k)¹ with the interface inertial term taken into account.¹⁵

The Green's function (23) determines the bare interaction of the instantons (which arise because n is an integer). Taking into account the mutual screening, we again obtain (in self-consistent approximation) a Green's function of the form given by Eq. (10) with G_0 from Eq. (23). Adding the k -independent self-energy part makes the energy of the step finite for all finite values of the parameters.

Nonetheless, the spectrum of excitations corresponding to the thus modified Green's function remains gapless. For the smallest k it lies slightly lower than the spectrum of the volume sound waves in the liquid $\omega = c_L k$. There is also an intermediate region in k space where this spectrum can be

approximated as $\omega \propto k^{1/2}$, whereas for $a^{-1} \gg k \gg \xi^{-1}$ the spectrum remains almost $k^{3/2}$.

The dilute instanton gas approximation is valid provided (1) the action S_1 corresponding to one instanton is large in comparison with unity, and (2) the wave function of the ground state is fairly well localized in the vicinity of the minima of the periodic potential $-A \cos(\varphi_j - \chi_j)$. For large enough A [when we can omit the first term in the square brackets in Eq. (23)] the magnitude of S_1 does not depend on A ,

$$S_1 \approx \frac{c^2 \hbar}{(J\rho_{\text{eff}} a^3)^{1/2} d}; \quad c_2 \sim 1 \quad (24)$$

and is sufficiently large if the magnitude of J in atomic units is small. For the QSOS model⁴ and the model of Section 1 the second condition is automatically satisfied in virtue of the first one. For the solid-liquid model considered the second condition is satisfied only if A is large in comparison with other characteristic energies. In the two interface models studied here, as in the QSOS model studied previously,⁴ the value of the action S_1 corresponding to one instanton is practically equal to half of the squared width of the surface. This is in agreement with the semiphenomenological statement by Fisher and Weeks³ concerning the width of the interface and the smoothness of the face. It is also important that instantons interact like charges (and not like, say, dipoles) and so can screen any distortion of the field n .

In the limit of an almost absolutely smooth surface (large J) we again can use perturbation theory, which enables us to show that the excitation spectrum has a gap.

A different form of the spectrum for different magnitudes of J indicates that the model displays a phase transition. This phase transition also manifests itself in the different behavior of the equal-time correlation function $\langle n_j n_l \rangle$ for $|r_j - r_l| \rightarrow \infty$.

For $J \gg A$ (when perturbation theory is applicable) it is more convenient to calculate this correlation function directly (without performing the Fourier transformation). In this case it decays exponentially. In the opposite limit of small J (when we can use the dilute instanton gas approximation) we must calculate $\langle n_j n_l \rangle$ with the help of Eqs. (10) and (23). Thus a power decay law is obtained. The origin of such behavior is accounted for by gapless excitation and the corresponding branching points in the denominator of $G(k, \omega)$.

The equal-time correlation function can also be found for nonzero temperature. It is easy to show that the power decay law becomes an exponential law. The coefficient in the exponent turns out to be proportional to the temperature (in the previously gapless region). This becomes clear

if one considers different terms of the sum over ω_l . Thus the difference between the phases vanishes at $T \neq 0$.

So it seems that the phase transition considered above exists (as a singular point of the free energy) only at zero temperature.

5. CONCLUSION

For all quantum models considered the faces of the crystal are smooth at zero temperature. The quantum effects do not change the temperature of the roughening transition considerably compared to its classical value. However, they can strongly increase the correlation radius ξ of the zero-frequency correlation function. This is of great importance for the experimental observation of faceting.^{2,17-20}

The size ε of a flat facet on the crystal surface is determined by the energy of the step on that facet.²¹ The energy of the step is inversely proportional to the correlation radius.^{4,22,23} Combining all these results, we get $\varepsilon = JL/\tilde{\alpha}\xi d \approx dL/\xi$, where $\tilde{\alpha}$ is the effective surface tension and L is the size of the crystal. Since the observation of a flat facet is impossible if its size is smaller than the correlation length, we obtain the condition $\xi \ll \xi^* \approx (dL)^{1/2}$. For the typical values²⁰ $L \approx 10^{-1}$ cm and $d \approx 10^{-8}$ cm we get $\xi^* \approx 10^{-4}$ - 10^{-5} cm. Due to the exponential growth of ξ with decreasing J , this may be a serious constraint for faces with large and even moderate Miller indices, since J is rapidly decreasing.

The freezing-melting waves were first proposed by Andreev and Parshin¹ as specific excitations for quantum rough faces. Assuming that the model of Section 4 is valid for real ${}^4\text{He}$, we still have two possibilities for observing freezing-melting waves even if all the faces are smooth at zero temperature. The first (trivial) one is the observation of such waves on a thermally rough interface (for $T > T_R$). The second (and more interesting) one is the observation of waves on a smooth interface, which can exist in the case of small J and large A . This second type of wave has a different type of spectrum for small k .

In the case of a quantum crystal existing at zero pressure or in the case when there is only quantum hopping of atoms along the interface, apart from the classical roughening we have a transition to the superfluid surface phase—a phase with nondissipative surface mass current. It is interesting that this transition does not depend on the atomic statistics. In that case gapless excitations of the surface occur with an acoustical type of spectrum.

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