Phase transitions on the surface of a quantum crystal

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A quantum model of a crystal surface is investigated. The phase diagram is constructed. A model of the interface between the quantum crystal and a quantum liquid, which takes into account the motion of the liquid, is formulated and investigated.

The recent widespread interest in the surfaces of quantum crystals has been stimulated to a large extent by Andreev and Parshin,[1] who, in addition to predicting the melting waves, also hypothesized the existence of the quantum rough faces at zero temperature. This hypothesis was criticized by Fisher and Weeks,[2] on semiphenomenological grounds.

The simplest model of a quantum interface, which corresponds to an identical density in the solid and liquid phases, was also constructed and investigated by Fradkin[3] and the present authors.[4] It was shown that at zero temperature the face is in a smooth state, and the change in the temperature of the transition to a rough state, T_R, as a result of quantum effects is small.

This paper is concerned with an investigation of more realistic models which describe the following features: 1) the free surface of a quantum crystal (existing in the absence of pressure) and 2) the interface between a quantum crystal and a quantum liquid.

The quantum model of the free surface of a crystal, which was formulated by Fradkin,[3] is described by the Hamiltonian

$$H = \sum_{(jj')} \left[\frac{I}{2}(\hat{n}_j - \hat{n}_{j'})^2 - \mu\cos(\phi_j - \phi_{j'})\right]; \quad \hat{n}_j = -i\frac{\partial}{\partial\phi_j}, \tag{1}$$

where the summation extends over pairs of nearest neighbors on a flat lattice, while the angular variables ϕ_j are associated via a Fourier expansion with the integer variables n_j, which represent the height of the surface. The first term in (1) is the energy associated with the differences between the heights at neighboring points on the surface and the second term describes hops of atoms along the surface (increase of n_j by 1 at one site with a simultaneous decrease by 1 at a neighboring site).

Fradkin investigated a sine-Gordon model, whose symmetry coincided with that of (1) and he showed that at $T = 0$ the surface is smooth, whereas T_R does not depend in leading order on μ.[3]

We note that Hamiltonian (1) has not only discrete symmetry associated with the shift in all n_j but also a continuous symmetry associated with the rotation of all ϕ_j. It follows that in addition to the transition from the rough state to the smooth state (which represents the spontaneous breaking of the first of the symmetries indicated) in

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the model examined, there can also be a phase transition due to breaking of the continuous symmetry. This transition becomes obvious at $J = 0$, when Hamiltonian (1) transforms to the Hamiltonian of the classical XY model.

We shall now examine the case of zero temperature. At $\mu \ll J$, using the perturbation theory it is easy to show that the excited states are separated from the ground state by a gap of width $(z/2)[J - \mu + O(\mu^2/J)]$ (z is the number of nearest neighbors).

In the reverse limit $\mu \gg J$, we can, by using the method described in Ref. 4, go over to a rarefied Coulomb gas of instantons, which will allow us to find the Green's function (correlation function) for surface oscillations $G(\mathbf{k},\omega) = \langle n_{\mathbf{k}\omega} n^*_{\mathbf{k}\omega} \rangle$. In the self-consistent approximation (whose accuracy increases with the ratio $\kappa = \mu/J$) for small values of k we would have

$$G(\mathbf{k}, -i\omega) = \frac{\hbar}{J(\xi^{-2} + k^2) + (\mu k^2)^{-1}\,\omega^2}\,, \tag{2}$$

where the momentum k is measured in units of inverse lattice constants a^{-1}, and $\xi^{-2} \propto \exp\left[-(c_1/2)\sqrt{\mu/J}\right]$ is proportional to the density of instantons. It follows from (2) that long-wavelength oscillations of the surface have a gapless spectrum (linear for values of small k). We note that the absence of a gap in the spectrum does not necessarily indicate that the surface is in a rough state. As demonstrated in Ref. 4 for a model of the type (1), the energy of the step is determined by the correlation function at zero frequency and in the case of the correlation function of the form (2), it is proportional to J/ξ.

The different form of the spectrum in different regions with respect to κ leads to the conclusion that a phase transition occurs at a critical value of κ_c. A study of the correlation functions $\langle \cos(\phi_j - \phi_l) \rangle$ in the limit $|r_j - r_l| \to \infty$ in the limiting cases $\kappa \gg 1$ and $\kappa \ll 1$ leads to the conclusion that it is the same transition that occurs in the XY model (i.e., at $J = 0$, $T \neq 0$). In the XY model the phase transition occurs when the free energy of the vortex vanishes. In the case $J \neq 0$, the possibility of a phase transition even at zero temperature can be explained by the fact that the vortex attracts instantons and as κ decreases the total energy of interaction with the instanton gas (which diverges logarithmically) cancels the self-energy of the vortex (which also diverges logarithmically).

Thus the phase-transition surface, which begins on the straight line in the plane (T,μ), terminates on the straight line in the plane (J,μ). One possible form of the phase diagram is illustrated in Fig. 1. Phases 1 and 2 are smooth, whereas phases 3 and 4 are

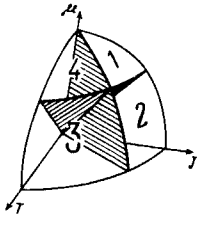

FIG. 1. Phases (4, 3) are rough; phases (1, 2) are smooth. Phases (1, 4) correspond to a finite superfluid density and can have nondissipative mass flow along the crystal surface.

rough. Phases 1 and 4 are superfluid, i.e., nondissipative mass flow along the surface, determined by $\nabla\phi$, with finite superfluid density ρ_s is possible. It has not been ruled out that the line of existence of the four phases is in reality split into two triple lines.

We shall now proceed to the quantum description of the interface between the solid and liquid superfluid phases. The model of such an interface examined in Ref. 4 is applicable when the densities of both phases are identical. To construct a general model we must take into account the presence of a phase factor, which depends on the phase of the condensate in liquid ^{4}He, in the amplitude of the transition of atoms from one phase to the other. Assuming that the phases are linearly related we obtain the Hamiltonian

$$H=\frac{J}{2}\sum_{(jj')}(n_j-n_{j'})^2-\mu\sum_j\cos(\phi_j-\lambda\chi_j)+\int[\rho_L\frac{\hbar^2}{2m^2}(\vec{\nabla}\chi)^2+\frac{c^2}{2\rho_L}(\delta\rho)^2]\,dV, \quad (3)$$

where χ_j is the phase of condensate at the site j on the interface (assuming that χ remains virtually constant within the limits of a cell) and $\delta\rho,\chi$ form a pair of Hamiltonian conjugate quantities. The volume integral gives the energy of the liquid, c and ρ_L are respectively the velocity of sound and density of the liquid and m is the mass of ^{4}He atoms. The law of conservation of matter at the interface determines uniquely the quantity $\lambda=(\rho_S-\rho_L)/\rho_S$, where ρ_S is the density of the solid phase.

The second term in the Hamiltonian has a simple physical meaning: when an atom leaves the crystal, the density of the liquid increases only by the amount $\Delta\rho=\rho_S-\rho_L$, because its boundary is displaced at the same time.

For small values of μ we can use, as in the preceding model, the perturbation theory and show that the spectrum of excitations has a gap. For sufficiently large values of μ we can use the saddle-point method, transform to a rarefied instanton gas and find the Green's function

$$G(\mathbf{k},-i\omega)=\frac{\hbar}{J(\xi^{-2}+k^2)+[\hbar^2\mu^{-1}+\rho_{ef}(k^2+\omega^2/c^2)^{-1/2}]\omega^2}\;;\;\rho_{ef}=\frac{(\Delta\rho)^2m^2}{\rho_L\rho_S^2\,a}, \quad (4)$$

whose poles describe the spectrum of excitations of the surface, which is gapless and which in the limit $k\to0$ approaches from below the spectrum of acoustic waves in the liquid $\omega=ck$. We note that in the limit $\xi^{-2}\to0$ (the vanishing instanton density), this spectrum transforms to the spectrum $\omega\propto k^{3/2}$, which coincides with the spectrum of melting waves.[1]

The different shapes of the spectrum, depending on the magnitude of μ, leads us to conclude that there is a phase transition in this model (at zero temperature), which does not correspond to a transition to the rough phase. Thus, in these models zero temperature corresponds to a smooth state with finite energy of the step, in agreement with the results of preceding studies.[2-4] In spite of this, circumstance at quantum transition frequencies higher than the critical frequency a phase transition of a different nature occurs and gapless excitations corresponding to the melting waves appear.

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