# Quantum effects in a faceting transition

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A quantum-mechanical model is developed for the interface between a crystal and a superfluid liquid. Quantum effects cannot cause a transition of facets or a rough state at absolute zero.

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Frank, Burton, and Cabrera[1] originally offered a thermodynamic model for the transition of a crystal facet from a smooth phase to a rough phase. It was later shown that this model has properties similar to those of the two-dimensional $XY$ model.[2] In this model, the energy of a facet depends exclusively on its configuration, i.e., on its potential energy $U(\{n_k\})$, where $n_k$, the height of the surface above some reference level, is expressed in discrete units on the order of the lattice constant, and the index $k$ specifies the site in the two-dimensional lattice on the facet. At zero temperature, $U$ has a minimum corresponding to $n_k = \text{const}$, and any facet is smooth, according to this model.

Andreev and Parshin[3] have suggested that quantum-mechanical effects could give rise to rough facets at zero temperature. A recent theoretical paper by Fisher and Weeks[4] has cast doubt on this suggestion. It is argued that the mean square of the zero-point vibrations of the surface converges, so that the positions of the surface cannot be sensitive to the atomic structure, and $U$ must change in discrete amounts.

In this letter we offer and analyze a quantum-mechanical physical model for the interface between solid and superfluid $He_4$.

Since helium atoms tunnel from the liquid to the crystal surface and back, the Hamiltonian of the system contains a matrix element which describes transitions between different configurations of the surface. We restrict the present discussion to transitions which change the number of atoms by one, and we assume that the magnitude of this matrix element does not depend on the configuration itself. This assumption is a good approximation for a facet with large Miller indices, which can be described in the classical approximation as a set of steps with large distances between jogs ($L_1$ and $L_2$ in Fig. 1), since in this case the tunneling occurs primarily at the jogs. We assume that the wave function $\Phi$ of the system depends exclusively on the surface

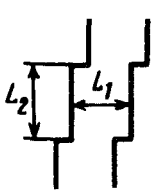


FIG. 1.

  

state, which is determined by the numbers $n_k$, and on the state of the superfluid liquid, which is determined by the velocity potential of the liquid, $\psi(x)$.

Because of the Bose condensate in liquid $He_4$, we need not be concerned about exact conservation of the number of particles. The part of the Hamiltonian describing the change in the surface configuration can thus be written

$$H_T = \sum_k \hat{\mu}_{0k} + \hat{\mu}_{1k} \left.\frac{\partial \psi}{\partial \nu}\right|_k + \text{H.a.}, \tag{1}$$

where the matrices $\hat{\mu}_{0k}$ and $\hat{\mu}_{1k}$ contain only elements with the change $n_k \to n_{k+1}$. The matrix $\hat{\mu}_{0k}$ corresponds to a transition to the condensate without a perturbation of the state of the liquid, while $\hat{\mu}_{1k}$ corresponds to an interaction with the hydrodynamic modes of the liquid. We have retained only the term with the normal velocity component, $(\partial\psi/\partial\nu)|_k$, at the boundary of the liquid, assuming that the other variables are inconsequential.

We must include in addition to $H_T$ in the Hamiltonian the energy of the liquid and the configurational energy of the surface, which we write as a quadratic function of the heights $n_k$; again, this is a good approximation for a facet with large Miller indices, and it is qualitatively correct for an arbitrary facet.[2]

We consider the case $\hat{\mu}_{0k} \neq 0$, $\hat{\mu}_{1k} \equiv 0$ here; we will discuss the distinguishing features of the opposite case $\hat{\mu}_{0k} \equiv 0$, $\hat{\mu}_{1k} \neq 0$ only in some concluding remarks. It is convenient to treat $\Phi(n)$ as the Fourier transform of the periodic function $\Phi(\phi)$, so that the Hamiltonian becomes

$$H = \sum_{k,k'} U_{kk'} (p_k - p_{k'})^2 + \mu_0 \sum_k \cos \phi_k, \quad p_k = -i \frac{\partial}{\partial \phi_k}, \quad \mu_0 > 0. \tag{2}$$

The extreme quantum limit corresponds to the case $\mu_0 \gg |U_{kk'}| \sim U$, when only the values of $\phi_k$ near the minimum of the cosine are important. Diagonalizing the corresponding quadratic Hamiltonian, we find a gapfree "phonon" spectrum at small wave vectors, $\omega_q \approx cq$. However, we must take into account the presence of many minima, since the result is of only zeroth order in the overlap integral (the tight-binding approximation).

To determine the nature of the spectrum we analyze the Feynman transition amplitude $Z(\phi, \phi', \theta)$ on a torus ($0 \leqslant \phi_k \leqslant 2\pi$) over a large imaginary time $\theta$ (see Ref. 5, for example):

$$Z(\phi, \phi' \theta) = \sum_{m_{k,j}} \int_0^{2\pi} d\phi_{k,j} \int_{-\infty}^{\infty} dp_{kj} \exp\left\{\sum_k 2\pi i m_{kj} p_{kj} - i p_{kj} (\phi_{k,j+1} - \phi_{kj}) - H(p_{kj}, \phi_{kj}) r\right\}, \tag{3}$$

where we have introduced the discrete time $\theta_j$ with a small step $\tau$, and $m_{kj}$ are integers. For large values of $\mu_0$, the following expression for the transition amplitude can be derived by the method of steepest descent:

$$Z \approx Z_0 \sum_{m_{kj}} \exp\left\{-\sum_{k,j,k',j'} m_{kj} m_{k'j'} G(\mathbf{R}_{kj} - \mathbf{R}_{k'j'})\right\}, \tag{4}$$

where $G$ is the Green's function on the space-time lattice corresponding to the expan-

sion of the Hamiltonian around the minimum, and $Z_0$ is the phonon partition function. It is easy to show that $G(0) \sim \sqrt{\mu_0/U}$, $G(R) \sim 1/R$ at large $R$. We thus have the partition function of a Coulomb gas of "instantons" with a low density $n_0 \sim \exp[-G(0)]$. According to the Debye-Hückel theory, the correlation functions of a gas of this sort fall off exponentially with a large but finite radius $R_c \sim \exp[1/2G(0)]$. This behavior corresponds to a gap in the spectrum of elementary excitations, $\omega_q^2 = c^2(R_c^{-2} + q^2)$, and to a smooth facet. There exists a slightly modified model, similar to the $XY$ model, for which separation (4) is exact.

In the case in which we have $\hat{\mu}_{0k} \equiv 0$, $\hat{\mu}_{1k} \neq 0$ in (1), we find precisely the same results with the corresponding Green's function $G$. The excitation energy for small $q$ is $\omega_q^2 = c^2 R_c^{-2} + \alpha q^3$, and the quantity $c^2 R_c^{-2}$ is exponentially small when $|\mu_{1k}|$ is large.

We have thus shown that for the models discussed here an arbitrary crystal facet (with its characteristic parameters $U$ and $\mu$) is absolutely smooth at zero temperature, despite the strong quantum-mechanical effects (except in the trivial case $U \equiv 0$), in accordance with the qualitative assertion of Fisher and Weeks.[4]

We might note that the convergence or divergence of the square of the zero-point vibrations does not itself play a role here. In the models which have been developed the reason for this situation is that the instantons are charged; in a one-dimensional spatial lattice the corresponding action is infinite, and there is no screening at large $\mu$. In general, however, there can be models for which the action is finite, even in the three-dimensional case, only for instantons with a zero net charge and in which there is no screening.

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