Quantum models of a crystal surface

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A very simple model for the surface of a quantum crystal, a generalization of the classical discrete Gaussian model, is proposed and analyzed. A transformation to an instanton gas shows that the surface is smooth for an arbitrary ratio of its parameters. Analysis shows that quantum effects cannot cause any substantial lowering of the temperature of the transition to a rough state. Another model proposed here for a crystal surface is of a type which has not been considered previously, in which the smooth state of the face is not absolutely stable in the absence of fluctuations. The phase diagram for the quantum version of this model is studied.

Burton and Cabrera[1] introduced the concept of a phase transition between rough and smooth states of a crystal surface more than 30 years ago. A theoretical understanding of the nature of the phase transition in the solid-on-solid (SOS) models was reached considerably more recently (see, for example, the review by Weeks[2]).

All the SOS models which have been studied to date have been definitely classical, i.e., nonquantum, models. A roughness transition has recently been observed experimentally for various faces of a ^{4}He crystal at equilibrium with a liquid (superfluid) phase.[3–7] In this case both the solid and the liquid are definitely quantum entities, so that quantum effects must be taken into account in a study of the phase transition and possible states of the surface. We do not believe that this topic has been studied adequately. In the only two places[8,9] where it has been discussed the authors have reaced diametrically opposite conclusions.

Andreev and Parshin[8] suggested that a rough surface state could be caused by quantum effects even at absolute zero. The basis for that suggestion was the possibility that the energy of a step on a crystal surface could drop to zero because of a quantum delocalization of jogs at the step. Generally speaking, it is not clear whether this approximation, which is based on the representation of an isolated step, is valid for describing a quantum-rough face, which is a conglomerate of mutually intersecting delocalized steps in various orientations.

Fisher and Weeks[9] have expressed a contrasting opinion regarding the role of quantum effects. Working from a finite surface width for an arbitrary power-law spectrum of surface excitations, they concluded that a rough surface structure could not exist at $T = 0$. They argue that a surface of finite width could not sense a periodic potential associated with the periodic structure of the solid. This argument, advanced without reference to any specific model, does not seem completely convincing. Furthermore, it does not rule out the possibility of a phase transition at $T = 0$. Fisher and Weeks use renormalization-group equations of the classical two-dimensional sine-Gordon model for an arbitrary nonzero temperature, without justifying the use of these equations at temperatures at which quantum effects would appear to be important.

Our purpose in the present paper is to resolve the role played by quantum effects in the roughening transition at a more concrete level. We construct and analyze some simple models for the interface of a quantum crystal and a quantum liquid, allowing for the possibility of quantum transitions between different surface states.

Some of the results derived here were reported in summary form in Ref. 10.

1. INTRODUCTION; CLASSICAL MODELS

In the conventional models a crystal with a free surface at equilibrium with its vapor is modeled by means of a lattice gas. It is assumed that a given site of this lattice can be occupied by an atom only if the site (or group of sites) directly below it is also occupied. This condition has given a name to an entire class of models (SOS models). Under this condition the state of a crystal with a free surface can be specified unambiguously by means of a two-dimensional matrix of integer variables which represent the height of the surface above some fixed level. The surface energy corresponding to the various surface configurations is specified as a function of these integer variables.

A representative model of this class is the discrete Gaussian (DG) model with the Hamiltonian

$$H_{\mathrm{DG}} = \frac{J}{2} \sum_{(ii')} (n_i - n_{i'})^2, \tag{1}$$

where the integer variables n_i are specified at the sites of a square plane lattice, and the summation is over pairs of nearest neighbors. It is assumed here and below that a factor of $\beta = (k_B T)^{-1}$ is incorporated in the definition of the statistical Hamiltonians. Model (1) describes the (001) face of a crystal with a simple cubic lattice.

Hamiltonian (1) is invariant under simultaneous displacements of all the variables: $n_i \to n_i + \Delta n$. This symmetry is preserved in the rough state of the surface, while the transition to the smooth state represents a disruption of this symmetry. Instead of directly studying the crystal properties of the DG and similar models, it is customary to perform a dual transformation[11,12] in the partition function

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$$Z_{\mathrm{DG}}=\sum_{n_i}\exp(-H_{\mathrm{DG}}), \tag{2}$$

converting this function into the partition function of the model of a planar magnetic material (an XY model). The nature of the phase transition in such models is well known and was first established by Berezinskiĭ.[13] The critical properties of such models can be analyzed by the method of renormalization-group transformations.[14] A convenient tool for analyzing the high-temperature properties of model (1) is to convert partition function (2) into the partition function of a lattice Coulomb gas.[15]

Another common approach is to replace Hamiltonian (1) by the sine-Gordon (SG) Hamiltonian

$$H_{\mathrm{SG}}=\frac{J^*}{2}\sum_{(ij)}(n_i-n_j)^2-Y\sum_i\cos 2\pi n_i, \tag{3}$$

specified for continuous variables n_i and having the same symmetry as H_{DG}. The sine-Gordon model (3) allows a renormalization-group analysis in both the Wilson[16] and field-theory[17] formulations.

The basis for replacing (1) by (3) is the identical symmetry of these Hamiltonians, i.e., the coincidence of their ground states[18,19] (at $T=0$).

There is an exactly solvable SOS model. This model was constructed by van Beijeren[20] for the (001) face of a crystal with a bcc lattice and is isomorphic to one version of the six-vertex model (F model) solved by Lieb.[21,22] All the models described above fall in the same universality class. A phase transition which occurs in them is of infinite order in the Ehrenfest classification. The rough phase is the line of critical points. The specific form of the structural features for quantities which are directly observable experimentally will be described in the following section.

For the classical thermodynamic SOS models the difference between the smooth and rough phases of the state of a two-dimensional surface is as follows: In the smooth state the surface has a finite width, and the fluctuations have a finite correlation radius. The free energy per unit length of the step is nonzero. The concentration of surface defects (outgrowths and pits) falls off rapidly (exponentially) as their size increases. In the rough state, in contrast, the free energy of a step vanishes, so that there can be defects of arbitrarily large size, including unclosed steps of infinite length. The fluctuations do not have a finite correlation radius, so that the width of the surface diverges.

We see that in the classical case the smooth and rough surfaces differ in many ways. In the quantum case (at $T=0$) the situation becomes slightly different. The free surface of a liquid (which, of course, could in no way be assumed atomically smooth) has a nonzero width. We assume that the free energy of a step is the basic characteristic of the smooth state. In this case the face can be represented by a plane region in the equilibrium faceting of the crystal.[23]

2. ROUGHENING TRANSITION AND FACETING OF A CRYSTAL

The transition of a face from a rough state to a smooth state corresponds to the appearance in the thermodynamically equilibrium shape of the crystal of a plane region corresponding to the given face. The size of this plane region is proportional to the jump ($\Delta\alpha'$) in the derivative of the surface free energy; in other words, it is proportional to the free energy per unit length of a step, F_{st} (Ref. 23). It has been shown[24,25] that for SOS models F_{st} is inversely proportional to the correlation radius of a dual model of the type of a planar magnetic material (see also Section 5). It then follows from the results of Kosterlitz[14] that near the transition point T_R the jump $\Delta\alpha'$ decreases to zero in accordance with

$$\Delta\alpha'\propto\exp\left(-b/(T_R-T)^{1/2}\right). \tag{4}$$

Unfortunately, experimental observations[3–7] of the appearance of plane regions on the surface of a ^{4}He crystal at equilibrium with a liquid (superfluid) phase have not yet made it possible to confirm or reject the behavior in (4).

There are certain other consequences of the theory of classical SOS models which can also be used for a comparison of experimental results with theoretical predictions.

The diagonal elements of the curvature tensor are inversely proportional to $\tilde\alpha=\alpha+\partial^2\alpha/\partial\chi^2$, where the angle χ is taken in the corresponding cross section, and α is the surface free energy. It can be concluded from both the renormalization-group analysis of the SG model[16] and the exact solution of the F model[20,21] that as the temperature tends toward the transition temperature T_R from above the quantity $\tilde\alpha$ remains finite but has a square-root anomaly:

$$\tilde\alpha(T)=\frac{k_BT_R}{h^2}\frac{\pi}{2}\left(1-\frac{(T-T_R)^{1/2}}{2b}\right), \tag{5}$$

where h is the interplanar distance, and b is the same constant as in (4). The universal relation for $\tilde\alpha(T_R)$ in (5) is analogous to the universal relation for the superfluid density at the transition point in the theory of superfluidity in thin films.[26] Fisher and Weeks[9] cited this relation as lower bound on T_R [i.e., an upper bound on $\tilde\alpha(T_R)$].

The exact solution of the F model[22] also suggests that at $T<T_R$ the following expression applies to the (still rough) faces making a small angle χ with the face at which the transition has occurred:

$$\tilde\alpha=D(T)\,|\chi|. \tag{6}$$

The same assertion is valid for the sine-Gordon model, as can be seen by making use of its equivalence to the massive Thirring model[27,28] and the known energy of the massive Thirring model with a finite soliton density.[29]

The intersection of the equilibrium form of the crystal with the plane perpendicular to the plane face is bounded by a line consisting of both smooth and curvilinear sections. Under condition (6) the shape of the curvilinear section of this line near the point at which it touches a smooth section is described by a parabola of degree 3/2.

Andreev's attempt[30] at a phenomenological description of the appearance of a plane region on the faceting leads to a functional dependence $\alpha(T)$ which has an anomaly corresponding to a phase transition on the surface described by Landau's mean field theory.[31b] The ordered phase is the high-temperature phase, according to the sign of the jump in the specific heat. In a two-dimensional system, however, Landau's theory has no range of applicability because of the governing role played by fluctuations.

3. SIMPLE QUANTUM MODEL FOR THE SURFACE OF A CRYSTAL

In the spirit of the SOS approximation we assume that in the case of an interface between a quantum crystal and a quantum liquid the state of the surface can be described by a wave function expandable in a basis of states with fixed values of n_i. We supplement the Hamiltonian of the DG model with terms corresponding to quantum tunneling between different surface configurations. For simplicity we assume that the amplitude of this tunneling, $\mu/2$, is independent of the initial and final states:

$$\hat{H}=\hat{U}+\hat{K}=\sum_{(ij)}\frac{J}{2}(n_i-n_j)^2-\frac{\mu}{2}\sum_i(a_i^++a_i^-). \tag{7}$$

The only nonzero matrix elements of the operators a_i^+ and a_i^- introduced here are the off-diagonal elements $\langle n_i+1|a_i^+|n_i\rangle=\langle n_i-1|a_i^-|n_i\rangle=1$. The kinetic energy of the proper motion of the liquid is not incorporated in Hamiltonian (7); this simplification is legitimate if the densities of the liquid and the crystal are the same. This model can also describe a domain wall in a magnetic material or a planar defect in a quantum crystal.

Like the classical Hamiltonian of the DG model, (1), Hamiltonian (7) can describe a variety of situations. First, it can describe the (001) face of a crystal with a simple cubic lattice. The variables n_i in this case represent the height of the surface (in units of the lengths of the lattice) and are determined on a square plane lattice. The operators a_i^+ and a_i^- make it possible for an atom to undergo a transition from the liquid to the crystal and vice versa at any site of this lattice.

The second situation is the (N1NM) face of a simple cubic lattice (or of some similar face), whose classical ground state is a regular lattice of jogs (Fig. 1). The variables n_i now represent the displacements of these jogs from certain fixed positions and are determined at the sites of the lattice of jogs, not on the original lattice. In the first term in (7), where the summation is over pairs of nearest neighbors, the interaction between neighboring jogs has been retained. The second term describes the tunneling of a jog to neighboring positions. The tunneling amplitude $\mu/2$, a characteristic of an isolated jog, can be assumed independent of n_i.

A similar Hamiltonian, but with an anisotropic interaction, can be used to model the $(10\,N)$ face for $N\gg1$. The classical ground state of such a face is a sequence of smooth steps separated by a distance N. The variable n_i in this case describes a deviation of a step from its regular position. One component of the two-component integer index i specifies the step; the other specifies the site on the step. The operators a_i^+ and a_i^- create and annihilate pairs of jogs and generate the motion of each of the jogs. An anisotropy of the interaction constants does not affect the nature of the conclusions which we can draw. If the differences n_i-n_j are very large, and the steps may collide, a quadratic increase in the energy as a function of n_i-n_j may be insufficient, and we have to assume that J increases in this case. It is intuitively clear, however, that such an "effective" increase in J could only make the faces "smoother" than in the model.

We use a standard procedure for transforming from the quantum model to a statistical model (see, for example, the review by Kogut[32]). For Hamiltonian (7) we construct an operator representing evolution along the imaginary time $-it$:

$$\hat{T}(t)=\exp\left(-\frac{t}{\hbar}\hat{H}\right)$$

$$=\lim_{\tau\to0}\left[\exp\left(-\frac{\tau}{\hbar}\hat{U}\right)\exp\left(-\frac{\tau}{\hbar}\hat{K}\right)\right]^{t/\tau}, \tag{8}$$

where

$$\hat{T}_U(\tau)=\exp\left(-\frac{\tau}{\hbar}\hat{U}\right)$$

is a diagonal operator, and

$$\hat{T}_K(\tau)=\exp\left(-\frac{\tau}{\hbar}\hat{K}\right)$$

splits up into the product of commuting factors,

$$\hat{T}_{K,i}(\tau)=\exp\left[\frac{\tau\mu}{2\hbar}(a_i^++a_i^-)\right].$$

Formally, $\hat{T}^*(\tau)\equiv\hat{T}_U(\tau)\hat{T}_K(\tau)$ differs from $\hat{T}(\tau)$ by terms of order τ^2 and higher, and in the limit $\tau\to0$ it becomes this operator. Straightforward calculations show that the matrix elements of the operators $\hat{T}_{K,i}(\tau)$ are

$$\langle n_i+p|\hat{T}_{K,i}|n_i\rangle=I_{|p|}(\tau\mu/\hbar), \tag{9}$$

where $I_{|p|}$ is the Bessel function of imaginary argument.

With the help of (9) we see that $\hat{T}^*(\tau)$ is the transfer matrix for the three-dimensional statistical model with the Hamiltonian

$$H^*=\frac{J\tau}{2\hbar}\sum_{(ij)}(n_i-n_j)^2-\sum_{(i,i+\tau)}\ln I_{|n_i-n_{i+\tau}|}\left(\frac{\tau\mu}{\hbar}\right). \tag{10}$$

The index i here is assumed to have three integer components, and $(i,i+\tau)$ denotes pairs of nearest neighbors (along t) which differ only in the third (temporal) component of the index i. The correspondence between the models with Hamiltonians (7) and (10) is established as $\tau\to0$.

Restricting the discussion to values of τ which satisfy the condition

$$\tau\mu/\hbar\gg1, \tag{11}$$

we can expand the logarithm of the Bessel function in (10) in

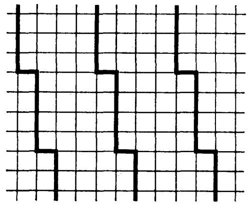


FIG. 1. The (N1NM) face ($N=4$, $M=4$) of a crystal with a simple cubic lattice—a lattice of jogs.

its index and transform to the anisotropic, discrete, three-dimensional, Gaussian Hamiltonian

$$H_{3DG}=\frac{J\tau}{2\hbar}\sum_{(ij)}(n_i-n_j)^2+\frac{\hbar}{2\tau\mu}\sum_{(i,i+\tau)}(n_i-n_{i+\tau})^2. \tag{12}$$

Chui and Weeks[15] have shown that the partition function of a discrete Gaussian model can be transformed into the partition function of a lattice Coulomb gas. In three dimensions, this gas has a finite chemical potential, and for arbitrary values of its parameters it is in a plasma state,[15] implying a smooth state of the original discrete Gaussian model.

Another approach to the study of Hamiltonian (12) is to transform to a sine-Gordon model with a continuous variable n:

$$S_{3SG}=\int d^2x\,dt\left\{\frac{J}{2\hbar}(\nabla n)^2+\frac{\hbar}{2\mu a^2}\left(\frac{\partial n}{\partial t}\right)^2-\frac{y}{a^2\tau}\cos 2\pi n\right\}. \tag{13}$$

Here and below, a is the lattice period. This substitution is justified best in the case $\mu \gg J$, in which there is in fact an interval of values of τ,

$$\hbar(\mu J)^{-1/2}\ll\tau\ll\hbar\mu^{-1},$$

which satisfy condition (12) and which are of such a nature that the coefficients of the sums in (12) are much less than unity. In this case, τ actually drops out of the problem: The coefficients of the squares of the derivatives in action (13) do not depend on τ. That no phase transition occurs in a model of this type can be shown by renormalization-group methods[33] with y assumed small.

These arguments still leave some doubt that the conclusions reached here also apply to the behavior of a model with Hamiltonian (10) in the case $\tau\to 0$. To eliminate this uncertainty we will show that the partition function (a functional integral) of the original model can be written as the partition function of a Coulomb gas even in the limit $\tau\to 0$, in which Hamiltonian (10) is substantially non-Gaussian, and the transformation of Chui and Weeks[15] cannot be used.

4. TRANSFORMATION TO A GAS OF INSTANTONS

Hamiltonian (7) is written in a form which implies that the wave functions depend on the variables n_i. To pursue the analysis, we transform from the integer variables n_i to angular variables φ_i, which take on values running over a circle and which are related to the n_i by a Fourier transformation. The n_i then become $-i\partial/\partial\varphi$, the a_j^+ become $e^{-i\varphi j}$, and the a_j^- become $e^{+i\varphi j}$, so that Hamiltonian (8) can be rewritten as

$$\hat{H}=-\sum_{(ij)}\left(\frac{\partial}{\partial\varphi_i}-\frac{\partial}{\partial\varphi_j}\right)^2-\mu\sum_i\cos\varphi_i. \tag{14}$$

This transformation is not the same as the dual transformation of Refs. 11 and 12, which sends the classical SOS model into the model of a planar magnetic material, in which the angular variables φ_j are defined on a dual lattice.

Hamiltonian (14) corresponds to the Feynman transition amplitude (in the Hamiltonian representation)

$$A[\varphi_{j'}(t),\varphi_j(0)]=\sum_{m_i(t')}\int_{-\infty}^{\infty}Dn(t')\int_{-\pi}^{\pi}D\varphi(t')\exp\left\{\frac{i}{\hbar}\int_0^t dt'\left[-\frac{J}{2}\sum_{(ij)}(n_i-n_j)^2+\sum_j(-\hbar n_j\dot{\varphi}_j+\mu\cos\varphi_j)\right]_{t'}+\sum_{i,t'}2\pi i n_i(t')m_i(t')\right\}, \tag{15}$$

where the summation over $m_i(t')$ makes the variables n_i discrete. The summation over $m_i(t')$ can be formally eliminated by transforming to the variables $\tilde{\varphi}_i=\varphi_i-2\pi m_i$, defined over the entire number line.

After a transformation to an imaginary time and a Gaussian integration over n_i, the dimensionless action in (15) becomes

$$S=\frac{1}{\hbar}\int_0^t dt'\left\{\int\frac{a^2d^2\mathbf{k}}{(2\pi)^2}U^{-1}(k)\,|\dot{\tilde{\varphi}}_k|^2-\mu\sum_i\cos\tilde{\varphi}_i\right\}, \tag{16}$$

Since we wish to show that the surface is smooth for arbitrary μ, we restrict the discussion to the limit $\mu\gg J$ and make use of the small value of the parameter J/μ.

$$U(k)=4J[\sin^2(ak_x/2)+\sin^2(ak_y/2)]\approx J(ak)^2.$$

Action (16) reaches its absolute maximum on trajectories with time-independent quantities $\tilde{\varphi}_i$ which minimize $-\cos\tilde{\varphi}_i$; for example, we could have $\tilde{\varphi}_i=0$ for all i. If we consider a single minimum and replace $-\cos\varphi_i$ by the parabola $\varphi_i^2/2-1$ (i.e., if we ignore the discrete nature of the situation), then the system can be broken up into several independent harmonic oscillators with a spectrum

$$\omega_{\mathbf{k}}=\hbar^{-1}[\mu U(k)]^{1/2}\approx ck,\qquad c=(J\mu)^{1/2}a/\hbar \tag{17}$$

(a nucleating spectrum without allowance for the discrete nature of the problem).

There are also trajectories on which action (16) reaches a local minimum. These trajectories connect different minima of the potential energy. On the simplest of them (i.e., those with the least action), the values of one of the variables (e.g., $\tilde{\varphi}_j$) at $t=+\infty$ and $t=-\infty$ differ by $\pm 2\pi$. The term $-\mu\cos\tilde{\varphi}_j$ in the potential energy (potential in the φ representation) on this trajectory goes through a maximum once. The other terms in the potential energy do not reach a maximum. We call such a trajectory an "isolated instanton." Because of the high barrier in the potential energy, the action corresponding to a single instanton is large.

We can introduce instantons in a more formal way by transforming to an imaginary time in functional integral (15) itself and evaluating the various terms of the sum over $m_i(t')$ by the method of steepest descent. The term for which all the $m_i(t')$ are zero gives us the trajectory on which the action reaches its absolute minimum.

An isolated instanton corresponds to a term in which only one of the quantities $m_i(t')$ becomes equal to ± 1 at one instant. Let us assume, for example $m_{i=0}(0)=+1$. By varying the corresponding action, we find equations describing the extremal trajectory:

$$i\frac{\partial\varphi_j}{\partial t}-\frac{J}{\hbar}\Delta^L n_j=2\pi i\,\delta(t)\,\delta_{j0}, \tag{18}$$

$$-i\frac{\partial n_j}{\partial t}+\frac{\mu}{\hbar}\sin\varphi_j=0, \tag{19}$$

where Δ^L is the lattice Laplacian. In (19) we replace $\sin\varphi_j$ by φ_j; this replacement is equivalent to an effective raising of the barrier height on the instanton trajectory. After this replacement, we can transform to a Fourier representation in the lattice and the time in (18) and (19), and we can easily find a solution of the resulting equations:

$$n(\mathbf{k},\ \omega)=2\pi iG_0(\mathbf{k},\ \omega),\quad \varphi(\mathbf{k},\ \omega)=2\pi i(\hbar\omega/\mu)G_0(\mathbf{k},\ \omega), \tag{20}$$

where

$$G_0(\mathbf{k},\ \omega)=\hbar[U(k)+M\omega^2]^{-1}\approx\hbar[J(ak)^2+M\omega^2]^{-1},\quad M=\hbar^2/\mu, \tag{21}$$

is the same as the nonrenormalized Green's function for the variables n, i.e., $G_0(\mathbf{k},\omega)=\langle|n_{k\omega}|^2\rangle_0$.

We should determine just what change is caused in the solution by the distinction between φ_j and $\sin\varphi_j$, which we have ignored. To resolve this point we put Eqs. (18) and (19) in the form

$$\operatorname{div}\mathbf{F}=(\mathbf{B}\nabla)\,\delta(\mathbf{X}), \tag{22}$$

in vector form in the three-dimensional space $\mathbf{x}$, where $\mathbf{x}=(\mathbf{r},\mathrm{t})$. Here

$$\mathbf{F}=\left(\frac{J\mu}{\hbar^2}a^2\nabla\sin\varphi,\frac{\partial}{\partial t}\varphi\right),\quad \mathbf{B}=(0.\ 2\pi).$$

Integrating (22) over the entire space, we find that the right side gives us zero. The integral of the left side reduces to an integral over an infinitely remote surface. Analogously, multiplying (22) by t, integrating, and making use of the explicit expression for $\mathbf{F}$, we find that the left side is again a surface integral over a remote surface. Everywhere on this remote surface we can replace $\sin\varphi$ by φ. The singularity on the right side of (22) thus unambiguously determines the solution at large distances, which turns out to be a dipole solution, in agreement with (20).

The distribution of the fields n and φ in the instanton, (20), which we have found explicitly can also be expressed in the coordinate representation. For example, as $t\to\pm\infty$ we have

$$n_{i=0}=\int\frac{a^2\,d^2\mathbf{k}\,d\omega}{(2\pi)^3}2\pi iG_0(\mathbf{k},\omega)\,e^{-i\omega t}\propto\frac{\hbar}{Jt}. \tag{23}$$

We can also use (20) to calculate the action corresponding to a single instanton, S_1. It turns out to be finite:

$$S_1=2\pi^2\int\frac{a^2\,d^2\mathbf{k}\,d\omega}{(2\pi)^3}G_0(\mathbf{k},\omega)=c_1\left(\frac{\mu}{J}\right)^{1/2},\quad c_1\sim1. \tag{24}$$

Since S_1 is finite, isolated instantons may exist. Under the condition $\mu\gg J$, their density (ν) in the three-dimensional space $(2+1)$ will be small. In leading order we have $\nu\propto\exp(-S_1)$ (see Ref. 34, for example).

The power-law decay of the field n in (23) indicates that the interaction of instantons must be taken into account. In the case of two instantons with charges $m_{1,2}=\pm1$, at the points $(R/2,\theta/2)$ and $(-R/2,-\theta/2)$, the solution is

$$n(\mathbf{k},\ \omega)=2\pi i[m_1\exp\{{}^1/_2 i(\mathbf{kR}-\omega\theta)\}+m_2\exp\{{}^1/_2 i(-\mathbf{kR}+\omega\theta)\}]G_0(\mathbf{k},\ \omega),$$

and the resultant action S_2 differs from $2S_1$ by the size of the instanton interaction:

$$W(\mathbf{R},\theta)=4\pi^2 m_1m_2G_0(\mathbf{R},\theta)\approx\frac{c_2m_1m_2\hbar}{[J(MR^2+J\theta^2)]^{1/2}},\quad c_2\sim1. \tag{25}$$

We see that the interaction of instantons in the three-dimensional space $\mathbf{X}$ with the metric $|X|=(\mathbf{r}^2+c^2t^2)^{1/2}$ falls off as $|X|^{-1}$ at large distances; i.e., at $\mu\gg J$ the instantons form a three-dimensional Coulomb gas, with a low density but a finite chemical potential. It follows from Debye-Hückel calculations (see Ref. 31a, for example) that a system of this type has a finite screening radius. This calculation can be reproduced quite easily in terms of Green's functions; the result is

$$G^{-1}(\mathbf{k},\omega)=G_0^{-1}(\mathbf{k},\omega)+\frac{4\pi^2\nu}{\hbar}\approx\frac{Ja^2}{\hbar}(c^{-2}\omega^2+k^2+\xi^{-2}), \tag{26}$$

where the instanton density ν should be expressed in terms of the complete Green's function,

$$\nu\propto2\exp[-2\pi^2G(\mathbf{r},\ t=0)], \tag{27}$$

and the correlation radius ξ satisfies the estimate

$$\xi\sim a\left(\frac{J}{\mu}\right)^{1/2}\exp\left[\frac{c_1}{2}\left(\frac{\mu}{J}\right)^{1/2}\right], \tag{28}$$

i.e., is exponentially large, by a factor proportional to the parameter μ/J.

A similar estimate of ξ can be found with the help of the sine-Gordon Hamiltonian in (13), through the use of a self-consistent equation for the Green's function[18] which differs from (26) only in the coefficient of ν.

We can thus conclude that for an arbitrarily large quantum tunneling amplitude $\mu/2$ the surface described by Hamiltonian (7) is smooth. That value of ξ which characterizes the scale dimensions at which the smoothness of the surface becomes significant increases rapidly with increasing μ/J. It also determines the size of the small gap in the surface excitation spectrum, $\omega^2=c^2(k^2+\xi^{-2})$.

Let us consider the problem of an artificially isolated step on the surface of a crystal. In other words, we seek the ground state of Hamiltonian (7) in the set of surface configurations which correspond to one of various versions of an infinitely long bent step with a given (average) orientation; we rule out the possible appearance of other defects. In the SOS approximation the problem then reduces to the one-dimensional version of Hamiltonian (7), where the variables n_i now represent the departure of the given section of the step from a fixed straight line. In this case the action corresponding to an isolated instanton diverges logarithmically. The interaction of instantons is logarithmic. The situation is completely analogous to a two-dimensional Coulomb gas, and as the parameter μ/J is changed there is a phase transition between smooth and rough states of the step. An increase in μ/J can make the energy of the rough (delocalized) step less than zero, as was pointed out by Andreev and Parshin. [8] Nevertheless, the analysis of the complete (two-dimensional) version of Hamiltonian (7) in this section shows that the reason for this conclusion is the neglect of fluctuations of the surface other than the bending of the given step. When these other fluctuations are taken into account correctly, an isolated step will still have a positive energy, despite its possible delocalization (at a large value of the ratio μ/J).

5. ENERGY OF A STEP

We showed in the preceding section that in the quantum SOS model (the QSOS model) the spectrum has a gap for any ratio μ/J, and the correlations fall off exponentially (there is a finite correlation radius). There can thus be no doubt that the state of the surface is smooth. This conclusion can also be reached by calculating the energy of a step, and this calculation is of interest in its own right.

A step of infinite length can be introduced only by means of boundary conditions at infinity, which are slightly inconvenient for an analysis. On a surface we can construct a step of finite length, however, for which we should introduce two screw dislocations of opposite sign. The change which arises in the partition function of the classical thermodynamic SOS model upon the introduction of a pair of screw dislocations of opposite sign can be seen particularly clearly after a transformation to dual displacements.[24,25] This change reduces to a multiplication of the partition function of the dual model by the correlation function for spins at the same points in the dual lattice as the screw dislocations: $\langle\cos(\varphi_j-\varphi_{j'})\rangle$. It follows immediately that the free energy per unit length of the step is T/r_c, where T is the temperature, and r_c is the correlation radius of the dual model.[24,25]

For this model we can directly express the energy of the step in terms of correlation functions.

In order to obtain a step of finite length we must introduce a mismatch on certain links; i.e., for these links we must replace the term $(1/2)J(n_j-n_{j'})^2$ in the Hamiltonian by $(1/2)J(n_j-n_{j'}+1)^2$. If we consider a step formed between screw dislocations at the points $(l+1/2, 1/2)$ and $(-l-1/2, 1/2)$, then we can choose the links with

$$j=(p,\ 1),\quad j'=(p,\ 0),\quad p=-l,\quad -l+1,\ldots,\ l-1,\ l,\tag{29}$$

as the set of links on which the mismatch is given. These links intersect the line segment connecting the points of the screw dislocations. Redefining the variables n_i, we can ignore the mismatch on any other set of links, which will now intersect that broken line through the dual lattice which connects the screw dislocations.

To introduce a mismatch on a set of links, as in (29), is equivalent to adding to Hamiltonian (7) a perturbation

$$V=V_1+V_2=J\sum_j f_jn_j+J(l+{}^1/_2),$$

where

$$f_j=\begin{cases}1 & \text{for } j=(p,1);\ p=-l,\ -l+1,\ldots,l-1,\ l\\ -1 & \text{for } j=(p,0)\\ 0 & \text{otherwise}\end{cases}.$$

The component V_2 increases the energy of the ground state by $J(l+1/2)$. To calculate the contribution of V_1 to the functional integral determining the ground-state energy, we expand the factor

$$\exp\left(-\int\frac{dt'}{\hbar}V_1\right)$$

in the functional integral in a Taylor series. The difference between the functional integral for the unperturbed Hamiltonian then reduces to multiplication by the series of correlation functions

$$\sum_{q=0}^{\infty}\frac{(-1)^qJ^q}{q!}\left\langle\left[\int\frac{dt'}{\hbar}\sum_j f_jn_j\right]^q\right\rangle_0,\tag{30}$$

taken for the *unperturbed* Hamiltonian.

For the rest of the calculations in this section of the paper we adopt the self-consistent approximation.[18] We assume that a correlation function of arbitrary order can be written as the sum of all possible products of binary correlation functions. Writing (30) in this form, we can sum the resulting series; we find

$$\exp\left\{\frac{J^2}{2\hbar}\sum_{ij}f_if_j\int dt'\int dt''\,G_{ij}(t',t'')\right\}.\tag{31}$$

The Green's function $G_{ij}(t';t'')$ in (31) depends on only the differences $i-j$ and $t'-t''$. In the argument of the exponential function in (31) we can single out a term which is proportional to the total time and to the length of the step (in the limit of a large length). Substituting expression (26) for G into (31) and integrating, we find

$$\begin{aligned}&-\frac{J}{2\hbar}\int\frac{dk_1}{2\pi}U(k_2=0,k_1)\,G(k_2,\omega=0,k_1)\\&\approx-\frac{J}{2}\left(1-\frac{1}{2}\frac{a}{\xi}\right).\end{aligned}\tag{32}$$

Taking into account the contribution of V_2 per unit length of the step, we find the energy of the step to be

$$E_{st}\approx J/4\xi.\tag{33}$$

For our QSOS model, $E_{\rm st}$ is proportional to $\exp\{-(c_1/2)(\mu/J)^{1/2}\}$ in the limit $\mu\gg J$, i.e., is finite for arbitrary μ.

In deriving (32) and (33) we have made use of only the explicit expression for the potential energy (in the n representation). The results thus apply not only to the QSOS model but also to other models of this type. It follows from the form of (32) that the energy of the step is finite not only because of the gap in the spectrum but also because of the finite correlation radius for the correlation function at a zero frequency. There can be no doubt that a calculation more rigorous than this self-consistent approximation will leave this circumstance fundamentally unchanged.

6. TRANSITION TEMPERATURE IN THE QSOS MODEL

We have thus shown that in this simple model quantum effects cannot lead to a roughness of the face at absolute zero. Nevertheless, at a large value of the parameter μ quantum fluctuations lead to a substantial increase (exponential in μ/J) in the correlation radius in comparison with atomic dimensions, and they lead to a decrease of the same magnitude in the gap in the surface excitation spectrum. Do these changes lead to an equivalent sharp decrease in the temperature of the transition to the rough state, T_R? An elementary analysis based on a comparison of the contributions of the energy and the entropy to the free energy of a step shows that the transition temperature is on the order of the energy of a segment of the step not of atomic length but of the minimum length which relatively straight segments of the step can have, i.e., ξ. In the product $E_{\rm st}\xi$ the factors which are exponential in S_1 cancel out, so that the relative decrease in T_R (if there is any such decrease at all) cannot be exponentially large.

The question of the transition temperature could also be approached within the framework of functional integration. The free energy at $T\neq 0$ can be expressed in terms of the Feynman transition amplitude over an imaginary time $-i\hbar/T$:

$$F=-T\ln\left\{\int D\varphi_j\, A\,(\varphi_j,\varphi_j,i\hbar/T)\right\}.$$

In this case the three-dimensional space in which we are considering the instantons coils up into a cylinder along the time coordinate. The gas of instantons becomes quasi-two-dimensional with a logarithmic long-range interaction.

The self-consistent equation for the Green's functions (26) (in which the frequencies should now be regarded as discrete: $\omega_n = 2\pi nT/\hbar$) can be used to find the temperature dependence of ξ and the transition temperature $T_R = (\pi/2)J$, which is independent of μ in this approximation. We know[14] that the renormalization of the interaction for the polarization of bound pairs of charges in a two-dimensional Coulomb gas leads to a value of T_R higher than $(\pi/2)J$. This increase, however, decreases with decreasing chemical activity of the Coulomb gas.

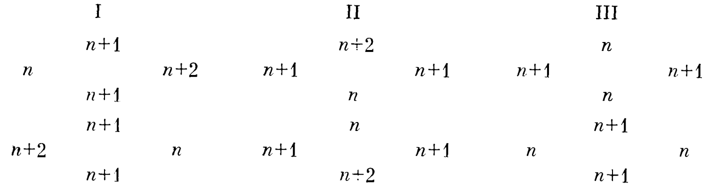
The chemical activity for a gas of instantons is proportional to $\exp\{-(c_1/2)(\mu/J)^{1/2}\}$ in the ultraquantum limit. It follows that in the limit $\mu\to\infty$ we have $T_R\to(\pi/2)J$. Accordingly, although quantum effects do lower T_R, the decrease could only be very slight. The critical behavior remains the same as in the classical case, but the range of applicability of limiting expressions such as (4) and (5) contracts with increasing μ.

7. AN ALTERNATIVE CLASS OF MODELS

It is not difficult to see that all the conventional SOS models[2] as well as the QSOS model discussed above have a property in common: The expression for the potential energy used in these models is such that in the absence of thermal fluctuations (and, in the present case, in the absence of quantum fluctuations) the planar state of the face under study is absolutely stable. In other words, the given face is present in the equilibrium faceting of the crystal. This is not the only possibility. If the long-range interaction of the links is ignored,[35] it would be completely permissible to have a situation in which some face of the crystal would be less favorable than a set of two or more faces of a different orientation, with the same projected area onto the plane of interest. The given face would then not be present in the equilibrium faceting of the crystal, and there would be a link or vertex.

An extremely simple classical model in which the planar state of a given face is not absolutely stable at $T=0$ can be constructed easily in the BCSOS model[20] for the (001) face of a bcc crystal. The surface state for this face is described in the SOS approximation by a set of integer variables defined on a square lattice which take on even values on one sublattice and odd values on another. A restriction imposed in the BCSOS model allows only the minimum difference in heights (± 1) between nearest neighbors. The energy of the surface configuration is determined by the difference in heights of the next-nearest neighbors.

Here are the six allowed configurations of a quartet of neighboring variables n_i:



With configurations I we associate a zero energy, with configurations II an energy ε, and with configurations III an energy E. van Beijeren, who constructed the BCSOS model,[20] showed that it is isomorphic with the six-vertex (6V) model. He discussed the case $\varepsilon = 0 > E$, in which an isomorphism with the symmetric antiferroelectric version of the 6V model (the F model) is achieved.

We would like to examine the case $E>\varepsilon>0$, which corresponds to the asymmetric ferroelectric version of the 6V model (which we will call the BCSOS/II model). The correspondence constructed by van Beijeren[20] means that we can use the known properties of the 6V model.[22] Reformulated in terms of the BCSOS model, these properties can be described as follows.

At $T=0$ a set of (101) and $(10\overline{1})$ faces would be preferable to the (001) face. Figure 2a shows the state of a crystal surface corresponding to the $(10\overline{1})$ face. According to this model, fluctuations would not be possible in this state, and its free energy would be zero at any temperature.

At $T=0$ there can also be a metastable surface state corresponding to the (001) face. This state is shown in the presence of a step in Fig. 2b. In this state any defect of finite

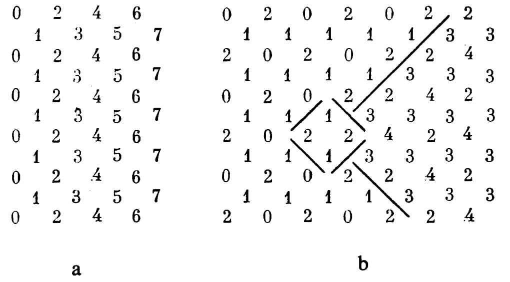


FIG. 2. Surface state of a bcc crystal. a—State corresponding to the $(10\bar{1})$ face; b—state corresponding to the (001) face (in the presence of a step with a jog).

size has a positive energy, but it is not absolutely stable since its energy, $\varepsilon/2$ (per vertex), is greater than zero. It can be seen from Fig. 2b that diagonally oriented steps do not increase the energy of the surface, and the energy of defects is associated with jogs on such steps. Accordingly, at any temperature $T>0$ there is some finite concentration of defects of arbitrarily large size. This means that a given state is rough at any $T>0$. As the temperature is raised, thermal fluctuations lower the free energy of the metastable state, and at a certain T_c $[T_c \sim E/\ln(E/\varepsilon)$ at $E \gg \varepsilon]$ the free energy vanishes. A phase transition occurs at this point.

At $T>T_c$ the thermodynamically most favorable state of the surface is that corresponding to a rough (001) face. A rounded region with a size which increases with increasing $(T-T_c)$ appears in place of a link on the equilibrium faceting.

We have thus constructed a BCSOS/II model in which a face of interest is rough at $T>T_c$, while at $T<T_c$ it is completely absent from the equilibrium faceting of the crystal. In the following section of this paper, we incorporate quantum fluctuations in this model.

It is not difficult to see that the energy of a step in a metastable state vanishes because the model ignores the interaction of more-remote neighbors. If we instead assume that the energy of a step is positive but much lower than T_c then there will be no changes in the results of this or the following section of the paper.

8. QUANTUM MODIFICATION OF THE BCSOS/II MODEL; PHASE DIAGRAM

We now incorporate in the model of the preceding section the possibility of a quantum tunneling with an amplitude μ. The restrictions imposed on the form of the potential energy are such that only transitions of the following type are possible:

$$\begin{array}{ccc} n & & n \\ & n+1 & \\ n & & n \end{array} \rightleftharpoons \begin{array}{ccc} n & & n \\ & n-1 & \\ n & & n \end{array} .$$

We assume $\varepsilon, \mu \ll E$, and we take the quantum tunneling into account by perturbation theory.

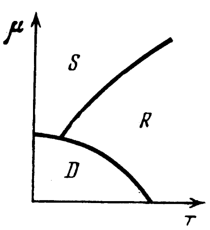


FIG. 3. Phase diagram for the quantum version of the BCSOS/II model. S—Region of a smooth state of the (001) face; R—rough state of the (001) face; D—region in which there is a link between the (101) and $(10\bar{1})$ faces.

In this model there can be no transitions from the state corresponding to the $(10\bar{1})$ face to any other states which have a finite number of altered heights n_j. The free energy of this state is zero at an arbitrary temperature. In contrast, the energy of a metastable state, E_b (Fig. 2b), is lowered by quantum fluctuations. The first nonvanishing correction arises in second-order perturbation theory. The energy can be written

$$E_b = \frac{\varepsilon}{2} - \frac{\mu^2}{2(4E-2\varepsilon)} + O\left(\frac{\mu^4}{E^3}\right). \qquad (34)$$

At $\mu > \mu_c \approx 2(E\varepsilon)^{1/2}$ the energy E_b obviously falls below zero, and the metastable state becomes absolutely stable. We might note that the presence of diagonally oriented steps (Fig. 2b) limits the possibilities of quantum transitions, so that such steps should be assigned a nonzero energy

$$E_{st} = \frac{\mu^2}{4E-2\varepsilon} + O\left(\frac{\mu^4}{E^3}\right). \qquad (35)$$

We must then conclude from general considerations that the surface state corresponding to the (001) face is rough only at a temperature $T>T_R \sim \mu^2/4E$, which may exceed T_c.

Working from estimates (34) and (35) we can construct a schematic phase diagram for the BCSOS/II model in terms of the coordinates T and μ (Fig. 3; for constants values of ε and E). Here S is the region in which the smooth state of the (001) face is stable, R is the rough state, and D corresponds to a decay into (101) and $(10\bar{1})$ faces. The line SR is a line of second-order transitions, while SD and RD are lines of first-order transitions.

According to this model, therefore, quantum tunneling leads to a slightly unexpected result: A smooth state of the (001) face becomes possible, and the temperature of the transition to the rough state increases (!) with increasing quantum tunneling amplitude μ. As in the QSOS model discussed earlier, there is no possibility of a rough face at absolute zero.

After this paper had been completed, we learned of work by Fradkin[36], who also constructed Hamiltonian (14) and studied its properties through the properties of the corresponding sine-Gordon Hamiltonian. We discussed the basis for a substitution of this sort in Section 3. Fradkin also reaches the conclusion that the surface is smooth at $T=0$.

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