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Roughening transition in quantum interfaces

Eduardo Fradkin
Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801
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The roughening transition in interfaces of quantum crystals and spin systems is studied. Quantum-mechanical solid-on-solid–like models are presented. I show that quantum interfaces of three-dimensional systems are generally smooth at zero temperature and display a classical roughening transition. In two dimensions, systems with discrete symmetry display a roughening transition at zero temperature.

The study of the properties of quantum interfaces has recently attracted considerable attention. A number of years ago, Andreev and Parshin[1] suggested that the surface of a quantum crystal, such as solid helium, may be rough down to zero temperature. This attractive idea has, however, been challenged more recently by experiments which suggest that these surfaces may be smooth at sufficiently low temperatures.[2,3]

In a recent Letter, Fisher and Weeks[4] have put forward an argument which indicates that the solid-fluid interfaces of quantum crystals should be smooth at very low temperatures. Using a coarse-grained Landau-Ginzburg-Wilson Hamiltonian to describe the dynamics of the interface, they showed that even if the interface is rough at finite temperature it is necessarily smooth at $T=0$.

In this Rapid Communication I study two models of quantum interfaces. These are quantum solid-on-solid–like models and are useful to discuss the classical-to-quantum crossover. My results agree with the conclusions of Fisher and Weeks. In particular, I show that the interfaces of *three-dimensional* quantum systems with long-range order are always smooth at $T=0$ for all values of the coupling constant. These results suggest that, at $T=0$, roughening can take place only if the bulk looses its long-range order. The interfaces of quantum two-dimensional systems may, in some cases, exhibit a roughening transition at $T=0$. The models discussed below apply to two types of systems: (a) solid-to-vacuum surfaces of quantum crystals and interfaces in quantum magnets with continuous symmetries (model I), and (b) interfaces of quantum spin systems with discrete symmetries. Although model I is not of the form of the Fisher-Weeks Hamiltonian, I show below that they are in the same universality class as far as their roughening properties are concerned. The details of the model are naturally different. In particular, while the Andreev-Parshin-Fisher-Weeks excitations have a spectrum $\omega \sim k^{3/2}$, for a solid-to-vacuum interface I obtain (model I) $\omega \sim k^2$ and for a magnetic interface $\omega \sim k$. These different properties, although important to the dynamics of these systems, do not change their equilibrium critical behavior.

I. THE MODELS

The first model (model I) I want to discuss describes the solid-to-vacuum surface of a quantum crystal. It turns out that it also describes the dynamics of an interface of an anisotropic spin-$\frac{1}{2}$ Heisenberg *ferromagnet*. Consider a three-dimensional cubic lattice with N sites and N/p ($p>1$) fermions. For the sake of simplicity I assume that the fermions, which represent the atoms, are spinless and have an attractive force between nearest neighbors of strength g. The fermionic character of the atoms is unessential in what follows and, in fact, will be safely replaced by bosons with an infinitely strong hard core. The Hamiltonian is

$$H=-K\sum_{\langle \vec{r},\vec{r}'\rangle}[c^{\dagger}(\vec{r})c(\vec{r}')+\text{H.c.}] -g\sum_{\langle \vec{r},\vec{r}'\rangle} n(\vec{r})n(\vec{r}') \ , \tag{1}$$

where the c's are either Fermi operators or bosons with hard cores and $n(\vec{r})$ is the local density. I will assume that the coupling constant g is much bigger than the hopping amplitude K. The sums of Eq. (1) run over nearest-neighbor sites on the lattice. This model gives a crude description of the quantum dynamics of a crystal of ^{3}He atoms, in a lattice-gas approximation, neglecting spin. The equivalency between fermions and bosons with hard cores in the strong-coupling limit makes this a model for ^{4}He crystals, too. Furthermore, Emery[5] showed quite generally that in the *strong-coupling limit* ($g \gg K$) the Hamiltonian of Eq. (1) is equivalent to that of an anisotropic spin-$\frac{1}{2}$ quantum *ferromagnet* ($g>0$) of the form

$$H_{\text{eff}}=-\frac{K}{2}\sum_{\langle \vec{r},\vec{r}'\rangle}[\sigma_1(\vec{r})\sigma_1(\vec{r}')+\sigma_2(\vec{r})\sigma_2(\vec{r}')] -\frac{g}{4}\sum_{\langle \vec{r},\vec{r}'\rangle}\sigma_3(\vec{r})\sigma_3(\vec{r}') \ . \tag{2}$$

The particle-number conservation symmetry of Eq. (1) turns into the conservation of $\sum_{\vec{r}}\sigma_3(\vec{r})$ in Eq. (2). It is worth mentioning that apart from the "hard-core" condition $\sigma_z^2=1$, Fermi statistics only contribute in higher orders in the strong-coupling expansion.

Let us now discuss a model for the interface itself. Let us first note that, in the classical limit ($g/K\to\infty$) the state of lowest energy is that which has an occupied close-packed set of N/p sites. For $p=2$ this is just a half-space and the system has a free interface. I can now imagine writing down an effective Hamiltonian describing the dynamics of the low-energy fluctuations of such an interface. Such a procedure can be carried out in the strong-coupling limit. The low-energy configurations of the interface are the traditional solid-on-solid type of the classical system.[6] Define an integer-valued height variable $n(x,y)$ at point (x,y). An in-

terface configuration is thus characterized by a set $\{n(x,y)\}$. A further, and minor, restriction is to impose that the difference in height between any two neighboring points be *at most* one. As usual, configurations with overhangs and islands are excluded. This defines the Hilbert space.

Quantum dynamics can be introduced by defining an operator $\hat{p}$ canonically conjugate to $\hat{n}$. Then I have

$$[\hat{n}(\vec{r}),\hat{p}(\vec{r}')]=i\delta_{\vec{r},\vec{r}'} , \tag{3a}$$

$$[\hat{n}(\vec{r}),e^{i\theta\hat{p}(\vec{r}')}]=-\theta e^{i\theta\hat{p}(\vec{r}')}\delta_{\vec{r},\vec{r}'} , \tag{3b}$$

and, if $|n\rangle$ represents an eigenstate of $\hat{n}$,

$$e^{i\theta\hat{p}}|n\rangle=|n-1\rangle . \tag{3c}$$

I can now write the effective Hamiltonian in the restricted Hilbert space. The result is, for model I,

$$H_{\rm I}=-K\sum_{\langle\vec{r},\vec{r}'\rangle}\cos[\hat{p}(\vec{r})-\hat{p}(\vec{r}')]+\frac{g}{2}\sum_{\langle\vec{r},\vec{r}'\rangle}|n(\vec{r})-n(\vec{r}')| , \tag{4}$$

which in the restricted Hilbert space is equivalent to

$$H_{\rm I}=-K\sum_{\langle\vec{r},\vec{r}'\rangle}\cos[p(\vec{r})-p(\vec{r}')]+\frac{g}{2}\sum_{\langle\vec{r},\vec{r}'\rangle}[n(\vec{r})-n(\vec{r}')]^2 . \tag{5}$$

This is the lattice Hamiltonian for model I.

Model II describes the dynamics of the interface of a quantum spin system with a discrete symmetry group. The prototype of such systems is the Ising model in a transverse field (ITF) whose Hamiltonian is equal to

$$H_{\rm ITF}=-K\sum_{\vec{r}}\sigma_1(\vec{r})-g\sum_{\langle\vec{r},\vec{r}'\rangle}\sigma_3(\vec{r})\sigma_3(\vec{r}') \tag{6}$$

and $g>0$ for a ferromagnetic interaction. For g bigger than some g_c this system has a ground state with long-range order. In this regime an interface may be forced on the system either by imposing antiperiodic boundary conditions or by changing the sign of the coupling constant g on a seam of bonds running across the system. The same arguments presented for model I yield a quantum solid-on-solid–like model with an effective Hamiltonian equal to

$$H_{\rm II}=-K\sum_{\vec{r}}\cos\hat{p}(\vec{r})+\frac{g}{2}\sum_{\langle\vec{r},\vec{r}'\rangle}[n(\vec{r})-n(\vec{r}')]^2 . \tag{7}$$

Notice that the models differ only by the form of the kinetic energy term. This reflects the different symmetry of the two models.

In order to proceed further it is convenient to make a continuum limit approximation. This is achieved by first softening the restrictions imposed on the Hilbert space and replacing the integer-valued states by regular bosonic states labeled by a field $\phi(\vec{r})$. The restriction to integers is imposed by a potential with a minimum on ϕ integer, e.g., $V(\phi)=u\cos2\pi\phi$.

In the continuum limit, the Hamiltonian of model I is

$$H_{\rm I}=\int d^2x\left[\frac{Ka^4}{2}[\nabla\Pi(\vec{x})]^2+\frac{g}{2}[\nabla\phi(\vec{x})]^2+\frac{u}{a^2}\cos2\pi\phi(\vec{x})\right] , \tag{8}$$

where a is a lattice spacing in the xy plane and $\Pi(\vec{r})$ is the momentum canonically conjugate to $\phi(\vec{r})$, i.e.,

$$[\phi(\vec{r},t);\Pi(\vec{r}',t)]=i\delta^{(2)}(\vec{r}-\vec{r}') . \tag{9}$$

Likewise, the Hamiltonian for model II equals

$$H_{\rm II}=\int d^2x\left[\frac{Ka^2}{2}\Pi^2(\vec{x})+\frac{g}{2}[\nabla\phi(\vec{x})]^2+\frac{u}{a^2}\cos2\pi\phi(\vec{x})\right] \tag{10}$$

in the continuum limit.

II. COULOMB-GAS REPRESENTATIONS

The roughening transition in classical interfaces can be understood by transforming into a Coulomb-gas representation.[7] The first step toward such a picture is the path integral. At $T=0$ I get

$$Z=\int D\Pi(\vec{x})\,d\phi(\vec{x})\,e^{iS} , \tag{11a}$$

where the action S equals

$$S=\int dt\left[\int d^2x\,\Pi(\vec{x})\frac{\partial\phi}{\partial t}(\vec{x})-H\right] . \tag{11b}$$

By integrating out the Π fields, one finds the effective Lagrangian

$$L_{\rm II}=\int d^2x\left[\frac{1}{2Ka^2}\left(\frac{\partial\phi}{\partial t}\right)^2-\frac{g}{2}(\nabla\phi)^2-\frac{u}{a^2}\cos2\pi\phi\right] \tag{12a}$$

for model II and

$$L_{\rm I}=\int d^2x\int d^2y\frac{1}{2Ka^4}\frac{\partial\phi}{\partial t}(\vec{x},t)\,G_0(\vec{x}-\vec{y})\frac{\partial\phi}{\partial t}(\vec{y},t)-\int d^2x\left[\frac{g}{2}(\nabla\phi)^2+\frac{u}{a^2}\cos2\pi\phi\right] \tag{12b}$$

for model I, where $G_0(\vec{x}-\vec{y})$ is the two-dimensional Green's function

$$-\nabla^2 g_0(\vec{x}-\vec{y})=\delta^{(2)}(\vec{x}-\vec{y}) . \tag{13}$$

The partition function of the quantum system at temperature $T=1/\beta$ is obtained by analytical continuation to imaginary time τ $(0\leq\tau<\beta)$,

$$Z\equiv{\rm Tr}e^{-\beta H}=\int D\phi\,e^{-S_E} , \tag{14}$$

where the field $\phi(\vec{x},t)$ is periodic in τ with period β and the Euclidean action S_E is, in terms of the dimensionless imaginary time coordinate $z=\tau\sqrt{gK}$, equal to

$$S_E^{(1)}=\int_0^{\beta(gK)^{1/2}}dz\left[\int d^2x\int d^2y\frac{1}{2a}\frac{\partial\psi}{\partial z}(\vec{x},z)\,G_0(\vec{x}-\vec{y})\frac{\partial\psi}{\partial z}(\vec{y},z)+\int d^2x\left[\frac{1}{2}(\nabla\psi)^2+\frac{u}{a^2\sqrt{gK}}\cos\bar{\beta}\psi\right]\right] \tag{15a}$$

for model I, where $\bar{\beta}=2\pi(K/g)^{1/4}$, and

$$S_E^{(\mathrm{II})}=\int_0^{\beta(gK)^{1/2}}dz\int d^2x\left[\frac{1}{2a^2}\left(\frac{\partial\psi}{\partial z}\right)^2+\frac{1}{2}(\nabla\psi)^2+\frac{u}{a^2K}\cos\bar{\beta}\psi\right] \tag{15b}$$

for model II, where $\bar{\beta}\psi\equiv 2\pi\phi$.

Thus the models under study are sine-Gordon-like on a $2+1$ cylinder of radius $\beta\sqrt{gK}$. As $T\to 0$, $\beta\sqrt{gK}\to\infty$ and I get the sine-Gordon model in three dimensions.

The Coulomb-gas representation can now be found with use of standard techniques.[7] Let $\{m(\vec{x},z)\}$ be a set of integer-valued degrees of freedom $(\pm 1,0)$ defined on the cylinder. The partition function is

$$Z=\int D\psi\, e^{-S_E(\psi)}=\int D\psi\exp\left[-K_0(\psi)+\int\frac{u}{a^2K}\cos 2\pi\psi\, d^2x\, dz\right]$$
$$\approx\sum_{\{m(\vec{x},z)\}}\int D\psi\exp\left[-K_0(\psi)+\int d^2x\, dz\left(\frac{2\pi i}{a^2}m(\vec{x},z)\psi(\vec{x},z)+\frac{m(x^2,z)}{a^2}\ln\frac{u}{2K}\right)\right], \tag{16}$$

where $K_0(\psi)$ represents the kinetic energy terms. By intergrating out the ψ fields I get the "Coulomb-gas" representation

$$Z=\sum_{\{m(\vec{x},z)\}}\exp\left[-\frac{1}{2}\sum_{j,k}m(\vec{x}_j,z_j)\,m(\vec{x}_k,z_k)\,V(\vec{x}_j-\vec{x}_k,z_j-z_k)\right]. \tag{17}$$

The effective potential V is different depending on whether $T=0$ or not and for the two models. At $T=0$ for model I, I get

$$V_{\mathrm{I}}(\vec{x}_j-\vec{x}_k,z_j-z_k)=\bar{\beta}^2G_{\mathrm{I}}(\vec{x}_j-\vec{x}_k,z_j-z_k)-\delta_{jk}\ln\frac{u}{2K},$$

where

$$G_{\mathrm{I}}(\vec{x}-\vec{x}',z-z')=\int\frac{d^2p}{(2\pi)^2}\int\frac{dp_z}{2\pi}\frac{\exp\{i[\vec{p}\cdot(\vec{x}-\vec{x}')+p_z(z-z')]\}}{p^2+p_z^2/p^2a^4}=\frac{\exp(-|\vec{x}-\vec{x}'|^2/4a^2|z-z'|)}{8\pi|z-z'|}, \tag{18}$$

while for model II one finds

$$G_{\mathrm{II}}(\vec{x}-\vec{x}',z-z')=a/4\pi(|\vec{x}-\vec{x}'|^2+a^2|z-z'|^2)^{1/2}. \tag{19}$$

Thus model II is exactly, at $T=0$, a *three-dimensional* Coulomb gas in an anisotropic space.

The effective potentials can be calculated just as easily at finite temperatures. The result, for both models, is

$$U(|\vec{x}-\vec{x}'|;z-z')\approx-\frac{2\pi}{\beta g}\ln\frac{|\vec{x}-\vec{x}'|}{a}+\text{core terms} \tag{20}$$

up to exponentially small terms in the limit $|\vec{x}-\vec{x}'|/a\gg[(\beta/4\pi)\sqrt{gK}\,]^{1/2}$ for model I and $|\vec{x}-\vec{x}'|/a\gg\beta\sqrt{g}K$ for model II.

Hence both systems become, at sufficiently long distances, equivalent to a two-dimensional Coulomb gas with a finite (periodic) extent into the third dimension. Notice that the argument of the logarithm does not depend on z, the imaginary time.

III. THE ROUGHENING TRANSITION

It is clear from the results of Sec. II that both systems have the same physics at finite temperature. As expected, both systems display a roughening transition identical to that of the classical interface models. This transition is well understood by now. It is of the Kosterlitz-Thouless type.[8] Quantum mechanics does not affect this behavior. Thus at temperatures lower than some critical value the interface (quantum or classical) is smooth. Furthermore, neither system shows a roughening transition at $T=0$ as a function of K/g. Using the Coulomb-gas picture we see that model II is, at $T=0$, equivalent to a *three-dimensional* Coulomb gas which Kosterlitz[9] has shown is always in a plasma phase and hence the interface is always smooth. In the case of model I the interaction energy, Eqs. (17) and (18), although highly anisotropic, is finite. Furthermore, the logarithmically divergent entropy contribution will always offset the energy and this system is also a plasma and hence the interface of a quantum crystal is always smooth at $T=0$. Only if the long-range order is lost does the interface become smooth. It is worth noting that the Fisher-Weeks[4] model has a representation very much like model I, Eq. (12b). The only change is to replace $G_0(\vec{x}-\vec{y})$ by

$$\int d^2\vec{k}\,\frac{e^{i\vec{k}\cdot(\vec{x}-\vec{y})}}{k^{1/2}}$$

which is finite. Thus the Fisher-Weeks model is always smooth at $T=0$ in agreement with the results of Ref. 4.

An important exception is the case of two bulk dimensions. As expected, both models are rough at *any* finite temperature. However, at $T=0$ model II is equivalent to a two-dimensional Coulomb gas which has a transition at some critical value of K/g. For K/g small the interface is smooth at $T=0$, but it is rough for K/g large. Thus an interface of a two-dimensional quantum spin system with discrete symmetry will display a roughening transition at $T=0$ as a function of K/g. This is, however, not the case for interfaces of quantum crystals since Eq. (18) is modified in two-dimensions by $(|z-z'|)^{1/2}$ in the denominator. The transition of model II may be exceedingly difficult to observe since this is an infinite order transition with an (infinitely) smooth specific heat.

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