Absence of domain wall roughening in a transverse-field Ising model with long-range interactions

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We investigate roughening transitions in the context of transverse-field Ising models. As a modification of the transverse Ising model with short range interactions, which has been shown to exhibit domain wall roughening, we have looked into the possibility of a roughening transition for the case of long-range interactions, since such a system is physically realized in the insulator $LiHoF_4$. The combination of strong Ising anisotropy and long-range forces lead naturally to the formation of domain walls but we find that the long-range forces destroy the roughening transition.

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I. INTRODUCTION

Magnetic systems present us with the opportunity to study not only classical but also quantum critical phenomena and thus provide us with unique insights in condensed matter physics and the intertwining of classical and quantum mechanics.[1] Of particular interest is the transverse field Ising model,[1–3] whose representation in terms of Pauli spin matrices is

$$H = \sum_{i,j}^{N} J_{ij}\hat{\sigma}_i^z\hat{\sigma}_j^z - h_x\sum_{i}^{N}\hat{\sigma}_i^x, \tag{1}$$

where h_x represents an applied transverse magnetic field and J_{ij} are coupling constants. Notice that in the absence of the magnetic field the Hamiltonian is diagonal in the $\hat{\sigma}^z$ basis, and the system is simply a classical Ising model. As the magnetic field is turned on, $\hat{\sigma}^x$ operators are introduced which do not commute with the $\hat{\sigma}^z$ operators. Thus, turning the transverse field on or off essentially turns quantum mechanics on or off in the system. The spins of this system align at temperature $T=0$ in a ferromagnetic ground state,[1] whereas at high temperatures the system becomes disordered. In the absence of a transverse magnetic field, a continuous phase transition occurs between the paramagnetic and ordered ferromagnetic states. This phase transition is driven by thermal fluctuations.

Applying a transverse magnetic field, $\mathbf{h}_x$, perpendicular to the axis of preferred magnetization, can also cause a transition between the ferromagnetic and the disordered states even at zero temperature.[1,2] This behavior is driven by quantum zero-point fluctuations of the z component of the spins due to the transverse field.

We now imagine the system described by Eq. (1) has domain walls—this is achieved in principle by imposing appropriate antiperiodic boundary conditions. It is expected that, in the absence of the transverse field, at $T=0$ the domain walls would be flat. As we increase temperature we would first observe nucleation of steps in the interface. At some temperature, called the roughening temperature T_R, the entropy of thermal fluctuations of the interface would dominate the interfacial energy and the interface would become rough.[4] At temperatures above the roughening transition, the amplitude of fluctuations in the surface's position scales as L^θ, where L is the system size and θ is an exponent characterizing the nature of the interface. Thus the interface fluctuations would diverge as the system length increases to infinity. However, we note that if $\theta<1$ then the system size would diverge faster than the fluctuations and so the fluctuations of the interface would not overwhelm the bulk order in the system. This would allow for a roughening transition to take place at a temperature lower than the bulk order-disorder phase transition temperature.

A physical realization of the transverse Ising model as described by Eq. (1) is provided by the insulating magnet[2,3] $LiHoF_4$. In this case, the coupling constants J_{ij} are actually no longer near-neighbor but dipolar in nature and so decay as the inverse distance cubed, $\sim 1/r^3$. In $LiHoF_4$ the Ho^{3+} ions are responsible for the magnetic behavior. The crystal field splitting of the Ho^{3+} states is such that the ground state is doubly degenerate and well below the higher states, thus leading to a very strong Ising anisotropy. The two spin states for each Ho^{3+} ion point along the z-axis, as shown in Fig. 1. The phase diagram, Fig. 2, is indicative of a quantum phase

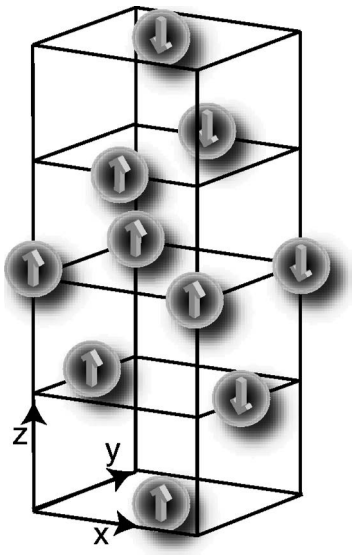

FIG. 1. $LiHoF_4$ behaves essentially as an Ising model with long range interactions. Interesting physics arises with the application of a transverse magnetic field.

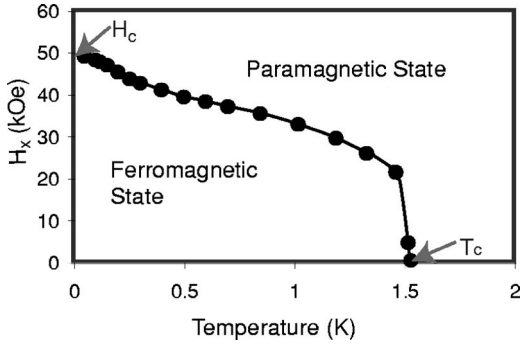

FIG. 2. $LiHoF_4$ undergoes both a classical thermal phase transition as well as a quantum phase transition with the application of a transverse magnetic field, after Ref. 2.

transition at $T=0$ and at a critical transverse magnetic field[2] $\mathbf{H}_x=\mathbf{H}_c\sim 49$ kOe, as well as a classical phase transition between ferromagnetic and disordered states in the absence of a magnetic field at $T_c=1.53$ K.

The dipolar long-range forces and the insulator nature of $LiHoF_4$ lead to the natural formation of needlelike alternating domains of antiparallel magnetization, without the need to force antiperiodic boundary conditions upon an experimental sample. Since $LiHoF_4$ is an insulator, the electrons and hence the constituent spins of the system are localized. The large anisotropy of the system means the domain walls which separate regions of opposite magnetization in a $LiHoF_4$ sample are sharp and well defined, in the sense that as we move across a domain interface the system abruptly switches from one magnetization state to another. This is to be contrasted to domain walls found in metals which are extended and provide for a continuous smoother transition of the magnetization as we move from one domain to the next. Thus, the first impression we get is that $LiHoF_4$ appears as an ideal system to study roughening transitions of domain interfaces. However, our analysis suggests otherwise.

In what folllows we first briefly review the case of only short-ranged exchange interactions being present, where we would expect to see a roughening transition, as described by Fradkin.[5] Then, we demonstrate that in the case of dipolar forces such as seen in $LiHoF_4$ the long-range nature of the interactions drives the roughening temperature up to the bulk transition temperature, so that the domain walls remain flat throughout the ferromagnetic regime. We show how to obtain a Hamiltonian for a field theoretical description of a single domain wall, which results in a modified sine-Gordon model that behaves as the regular sine-Gordon model but with effectively higher dimensionality. We see how this behavior is verified by a renormalization group calculation using a smooth cutoff and conclude that the effective higher dimensionality of the domain wall, $d>2$, indicates the absence of a roughening transition and the persistence of flat domain walls in the ferromagnetic phase. Finally, we mention some further considerations for stepped interfaces.

II. TRANSVERSE ISING MODEL WITH ROUGHENING: SHORT RANGE INTERACTIONS

Using an Ising model for a two-state spin system with appropriate boundary conditions, a two-region problem can be set up with an interface of finite width separating regions of opposite spin. Investigations of this interface for the case of short-range interactions show that it undergoes the roughening transition.[6–11] A numerical estimate for the roughening transition was carried out some time ago by Weeks *et al.*[12] for a 2D interface in a classical Ising model, obtaining a roughening critical temperature of $0.57T_c$, where T_c is the bulk critical temperature for the order-disorder transition. It would be useful to redo this calculation with higher precision using newer computational techniques.

In the case of two-dimensional interfaces it was proposed by Fisher and Weeks[13] that the interfaces of three-dimensional quantum crystals are always smooth at zero temperature. This suggests that there can be no quantum roughening transition. Fradkin[5] investigated the suggestion further and verified it for two different models, namely, a model describing the solid to vacuum interface of a three-dimensional quantum crystal, which is similar to the model used by Fisher and Weeks, and a model describing the interface of the three-dimensional quantum transverse Ising model. Fradkin obtains the effective Hamiltonian of the two-dimensional interfaces, both for the quantum crystal model,

$$H_{\mathrm{QC}}=-K\sum_{\mathbf{r}}\cos[\hat{p}(\mathbf{r})-\hat{p}(\mathbf{r}')]+\frac{J}{2}\sum_{\langle\mathbf{r},\mathbf{r}'\rangle}[n(\mathbf{r})-n(\mathbf{r}')]^2, \tag{2}$$

and for the transverse Ising model,

$$H_{\mathrm{TI}}=-K\sum_{\mathbf{r}}\cos\hat{p}(\mathbf{r})+\frac{J}{2}\sum_{\langle\mathbf{r},\mathbf{r}'\rangle}[n(\mathbf{r})-n(\mathbf{r}')]^2, \tag{3}$$

where $\hat{p}$ is canonically conjugate to n, the discrete height variable.

Notice here the difference in the kinetic energy term which arises from the difference in symmetry between the different models and gives rise to different dynamics.[5] For the quantum crystal model the particle number $N=\Sigma_{\mathbf{r}}n(\mathbf{r})$ is conserved while for the analogous quantity for the transverse Ising model it is not. Since our model for $LiHoF_4$ is the transverse Ising model we take into account the considerations by Fradkin[5] instead of the Fisher and Weeks model.[13]

The $2+1$ dimensional quantum interface model for the transverse Ising model is dual to a three-dimensional general Coulomb gas which is known to have only a conducting plasma phase.[14] Since the surface has to be smooth at $T=0$ this implies that roughening can only occur if the bulk loses its long-range order, so the critical magnetic field parameter for the roughening and order-disorder transitions will coincide, i.e., $h_R=h_c$.

For finite temperatures, where the transition is classical, we can ignore the cosine kinetic energy terms since these become unimportant, and notice that the two models in Eqs. (2) and (3) become the same, namely a realization of the discrete Gaussian SOS model.[5] A continuum version of the discrete Gaussian SOS model is the sine-Gordon model.[15] Briefly, the sine-Gordon model hamiltonian contains two terms:

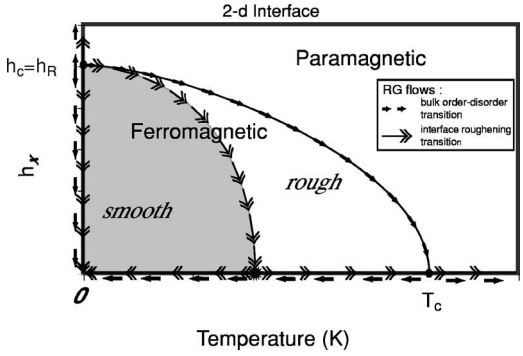

FIG. 3. For a two-dimensional interface we expect a thermal roughening transition at some finite temperature. At zero temperature the critical transverse field for the roughening transition coincides with that of the bulk order-disorder transition. The two sets of arrows indicate the expected qualitative renormalization group flows for the different phase transitions: the bulk order-disorder transition (plain arrows) and the interface roughening transition (double-headed arrows).

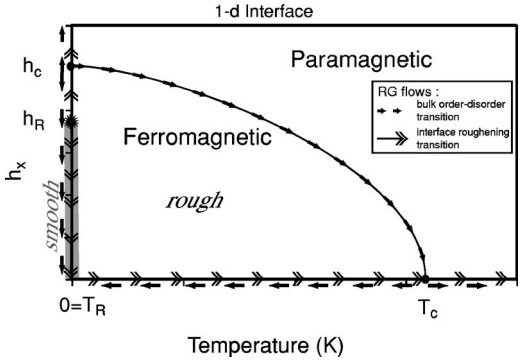

FIG. 4. For a one-dimensional interface the system is rough at all finite temperature. The roughening transition occurs at zero temperature. In addition we expect a quantum roughening phase transition. The two sets of arrows indicate the expected qualitative renormalization group flows for the different phase transitions: the bulk order-disorder transition (plain arrows) and the interface roughening transition (double-headed arrows).

$$H_{\mathrm{sG}} = \int d^2\mathbf{r}\left[\frac{J}{2}(\nabla n(\mathbf{r}))^2 - y\cos\left(\frac{2\pi n(\mathbf{r})}{a}\right)\right]. \qquad (4)$$

The first term describes the cost of local fluctuations of the interface. The second term takes the effects of the lattice into account, and the fact that the interface height field $n(\mathbf{r})$ can really only take discrete values, namely multiples of the lattice spacing a. This periodic term promotes the pinning of the interface onto equidistant parallel planes, and thus encourages the interface to remain smooth. The sine-Gordon model undergoes a Kosterlitz-Thouless phase transition[15,16] and displays two distinct phases corresponding to the smooth surface at low temperature, where the cosine term is perturbatively important, and a rough phase at high temperatures, where the cosine term is unimportant. Thus we expect a roughening phase transition at some finite temperature, T_R, less than the bulk order-disorder transition temperature. Given that the interface has to be smooth at $T=0$ we propose the phase diagram shown in Fig. 3, where we include, for completeness, the related renormalization group (RG) flows. For the two-dimensional interface we notice that in the temperature region $T_R<T<T_c$ the flows are opposite for the two different phase transitions. This is related to the fact that the onset of high fluctuation for the interface occurs at a temperature below the critical order-disorder transition where the bulk system loses its long-range order.

It is also interesting to consider a one-dimensional interface in the transverse field Ising model, in which case we expect the domain wall to be rough at any finite temperatures. However, as pointed out by Fradkin,[5] at zero temperature the transverse Ising model is dual to a two-dimensional Coulomb gas.[17] This is dual in the continuum limit to a two-dimensional sine-Gordon model and is known to have a metal-insulator phase transition[14,16,18] at some value of h_x at $T=0$: we expect a smooth interface for small h_x; as we increase h_x we go through a phase transition to a rough interface for some h_R, before the onset of the order-disorder transition at h_c. The proposed phase diagram and qualitative RG flows are shown in Fig. 4. We see that for the roughening transition, temperature is always a relevant parameter and flows to a fixed point at infinity.

III. $LiHoF_4$ TWO-DOMAIN SYSTEM: LONG-RANGE INTERACTIONS

As mentioned in the Introduction, the behavior of $LiHoF_4$ can be understood in terms of a quantum Ising model in the presence of a transverse magnetic field,[2,3] in which the states of the Ho^{3+} ions are represented by the Ising spins $|\uparrow\rangle$ and $|\downarrow\rangle$. The effective Hamiltonian looks like[3]

$$H = \frac{1}{2}\sum_{i\neq j} J\frac{r_{ij}^2 - 3z_{ij}^2}{r_{ij}^5} S_i^z S_j^z - h^x \sum_i S_i^x + \frac{1}{2}\sum_{\langle i,j\rangle} J_{\mathrm{ex}}\sigma_i^z\sigma_j^z, \qquad (5)$$

where h^x corresponds to an applied transverse magnetic field and J_{ex} is an effective antiferromagnetic exchange term that is added to obtain an effective Hamiltonian that matches the experimental results.

Since $LiHoF_4$ forms domains naturally, we consider for our calculations a system consisting of two semi-infinite three-dimensional domains of antiparallel magnetizations (directed in the positive or negative z-directions) that are separated by a domain wall set at $x=0$. We want to calculate the configurational energy for fluctuations in the domain wall with respect to a flat interface. We proceed by assuming a height for the domain interface to be a general function $\psi(y,z)$, so that the magnetization vector for the system becomes,

$$\mathbf{M} = \{0,0,m_0\,\mathrm{sgn}(x-\psi(y,z))\}. \qquad (6)$$

We consider the classical magnetostatic problem and after we relate a "magnetic charge density" $q(x,y,z)$ to the magnetization,

$$q(x,y,z) = -\nabla\cdot\mathbf{M}, \qquad (7)$$

we see that in analogy with electrostatics, the extra energy associated with having a nonflat profile is given in the continuum limit by[19]

$$U = \frac{1}{2}\int_V q(\mathbf{r})\phi(\mathbf{r}), \tag{8}$$

where ϕ is the magnetic potential given in three dimensions by

$$\phi(\mathbf{r}) = \int_{V'} \frac{q(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}. \tag{9}$$

This results in the following expression for our system:

$$U = 2m_0^2 \int dydzdy'dz' \times \frac{\partial_z\psi(y,z)\partial_{z'}\psi(y',z')}{[(\psi(y,z)-\psi(y',z'))^2+(y-y')^2+(z-z')^2]^{1/2}}. \tag{10}$$

We now assume that the profile of the interface does not vary greatly from one position to another and so we can expand the denominator to zeroth order in $[\psi(y,z)-\psi(y',z')]$, which is certainly true in the "smoother" regime of $\theta \ll 1$ and probably asymptotically correct for all $\theta < 1$. We can rewrite the energy in this approximation in Fourier space to obtain

$$U_0 = 4\pi m_0^2 \int \frac{dk_y dk_z}{(2\pi)^2}\frac{k_z^2}{|k|}|\psi(k_y,k_z)|^2. \tag{11}$$

Odd order terms vanish and higher even-order terms do not display the singular behavior of the zeroth-ordered term which will ultimately dictate the critical behavior of our system.

A point of concern here is that, in the continuum model used, the fluctuations in the y-direction do not have any energy cost since they do not change the angle between magnetization up and down in the z-direction as we move across the interface. Thus we should consider fluctuations in the y-direction in a lattice model rather than in the continuum to see their effect. A further complication arises, since in addition to the dipolar Ising model interaction which would raise the energy of the system there could be an effective exchange interaction in $LiHoF_4$ as indicated in Eq. (5), tending to lower the energy as the domain wall fluctuates. This effective exchange interaction has recently been discussed by Chakraborty *et al.*,[3] who obtained an estimate of J_{ex} from Monte Carlo simulations,

$$J_{ex} = 0.75J = 0.75 \times 0.214K. \tag{12}$$

To get a feel for the system stability to deformations and the domain wall surface tension we took a $LiHoF_4$ system starting with two semi-infinite domains of antiparallel magnetization (a cube with sides extending to $\pm N$) and then we introduced a semi-infinite unit step deformation in the chosen y-direction. Briefly, this is a lattice sum calculation where the dipolar interactions were summed over the infinite Bravais lattice, which for $LiHoF_4$ has tetragonal unit cells with dimensions $(a,a,c)=(1,1,2.077)a$, where $a=5.175$ Å is the lattice constant. Each unit cell has four spins, at the positions $\{0,0,0\}$, $\{0,a/2,c/4\}$, $\{a/2,a/2,-c/2\}$, and $\{a/2,0,-c/4\}$. The sums show slow convergence, $\sim 1/x^3$, so we used Ewald[20] summation to obtain faster convergence. Our results indicate that the deformation causes an increase in energy from the dipolar term of $\frac{1}{2}\times 2(2N+1)\times 0.927J$, whereas the exchange interaction would cause a decrease by $\frac{1}{2}\times 2(2N+1)\times 0.75J$. Thus, we have an overall positive energy cost to a single step deformation and a positive surface tension associated with this deformation. Taking the zeroth order term of the Hamiltonian Eq. (11) and following the above discussion of our numerical considerations for the deformation of an interface in equilibrium, we add an extra tension term, and consider the free interface to be modeled by

$$U_0' = 4\pi m_0^2 \int \frac{d^2\mathbf{k}}{(2\pi)^2}\left(\frac{k_z^2}{|k|}+\gamma a k^2\right)|\psi(\mathbf{k})|^2. \tag{13}$$

We note that at this Gaussian level the individual modes are not coupled and hence we can evaluate the average of U_0 assigning a variance of $1/2\beta$ to each mode. Thus we can write down the mean correlated height difference, G, as

$$G = \langle(\psi(y,z)-\psi(0,0))^2\rangle \tag{14}$$

$$= \int \frac{d^2\mathbf{k}}{(2\pi)^2}\frac{1-e^{i\mathbf{k}\cdot\mathbf{r}}}{4\pi\beta m_0^2\left(\frac{k_z^2}{|k|}+\gamma a k^2\right)}. \tag{15}$$

In the large distance limit, $G \sim O(L^0)$, thus indicating that the interface has bounded fluctuations and is smooth at all temperatures.

A. Long-range sine-Gordon model

We now wish to investigate any possibility of critical behavior, by performing a renormalization group analysis. Starting from the zeroth order term in our modified energy expression Eq. (13) we now include a sine-Gordon term to take into account the existence of the lattice and write the full action as

$$-\beta H_u = -\beta\left\{4\pi m_0^2\int \frac{d^2\mathbf{k}}{(2\pi)^2}\left(\frac{k_z^2}{|k|}+\gamma a k^2\right)\psi(\mathbf{k})\psi(-\mathbf{k}) - \frac{g_u}{a^2}\int d^2\mathbf{r}\cos\left(\frac{2\pi\psi(\mathbf{r})}{a}\right)\right\}, \tag{16}$$

where $\beta=k_BT$, a is a lattice constant, and γ and g_u are couplings for the surface tension term and fugacity of the system, respectively. To make the coupling constants dimensionless we take $\beta m_0^2 \to m^2/a^3$, $\beta g_u \to g$, and in addition we define a dimensionless field in real space,

$$\phi(\mathbf{r}) = \frac{2\pi\psi(\mathbf{r})}{a}, \quad \phi(\mathbf{k}) = \frac{2\pi}{a}\psi(\mathbf{k})$$

so that our action becomes

$$S = -\frac{m^2}{\pi}\int \frac{d^2\mathbf{k}}{(2\pi)^2}\left(\frac{k_z^2}{a|k|}+\gamma k^2\right)\phi(\mathbf{k})\phi(-\mathbf{k}) + \frac{g}{a^2}\int d^2\mathbf{r}\cos(\phi(\mathbf{r})). \quad (17)$$

The above action is just the familiar sine-Gordon field, with an extra coefficient $k_z^2/a|k|$ in the quadratic part, which accounts for the long range nature of the interactions. The sine-Gordon model can be renormalized via a smooth cutoff approach.[18] Note here that if we now try to renormalize the above action using standard isotropic rescalings then the end result is that the singular $\sim k_z^2/a|k|$ term cannot be renormalized and will dominate—since the renormalization of nonsingular couplings cannot generate singular terms. Therefore, let us consider a different rescaling for the x and y directions while, as is usual, also requiring that the field $\phi(\mathbf{r})$ does not change under rescaling so as to preserve the lattice structure. We rescale so that $z'=e^{-bs}z$, $y'=e^{-\alpha s}y$, $k_z'=e^{bs}k_z$, $k_y'=e^{\alpha s}k_y$, $\phi'(\mathbf{k}')=e^{-(b+\alpha)s}\phi(\mathbf{k})$, and $g'=e^{(b+\alpha)s}g$, where $\alpha, b \geqslant 0$.

We concentrate on the terms quadratic in the field and choose a and b so that the two terms in the quadratic prefactor scale the same way under the transformation. This cannot be done consistently unless we assume $\alpha < b$ which leads to the choice $\alpha=\frac{2}{3}b$. We choose $\alpha=1$ and notice that terms which behave as k_z^2 become irrelevant in this RG scheme.

Bearing in mind the above discussion and in addition introducing a smooth momentum cutoff function $f(k_y,k_z)$ in the simplified action to take the effects of the lattice into account, we finally obtain the rescaled action

$$S = -\frac{m^2}{\pi}\int \frac{d^2\mathbf{k}' e^{s/2}}{(2\pi)^2 f(k_y,k_z)}\left\{\frac{k_z'^2}{a|k_y'|}+\gamma(k_y'^2)\right\}|\phi'(\mathbf{k}')|^2 + \frac{g e^{5s/2}}{a^2}\int d^2\mathbf{r}\cos(\phi(\mathbf{r})). \quad (18)$$

This has the form of the original hamiltonian if we define our new couplings as

$$g' = e^{5s/2}g, \quad (19)$$

$$m'^2 = e^{s/2}m^2, \quad (20)$$

and the new cutoff function

$$f'(k_y',k_z') = f(k_y,k_z) = f(e^{-s}k_y', e^{-(3s/2)}k_z'). \quad (21)$$

We try to pick the cutoff function in a way consistent with the spatial anisotropy of the problem, and also for future convenience. One reasonable choice is

$$f(k_y,k_z) = e^{-a^2(k_z^2+\gamma a|k_y|^3)}. \quad (22)$$

The RG calculation (described in more detail in the Appendix) now proceeds as usual[18] though we notice straight away that we have scaling of the temperature even before we go to higher order terms. Thus, even though we are looking at a 2D problem we have effectively higher dimensional behavior. As is known[14] the Ising model is equivalent to a Coulomb gas in all dimensions and this is always in the plasma phase for $d>2$. Our final results from the perturbative renormalization group to first order in g yield the following differential renormalization equations

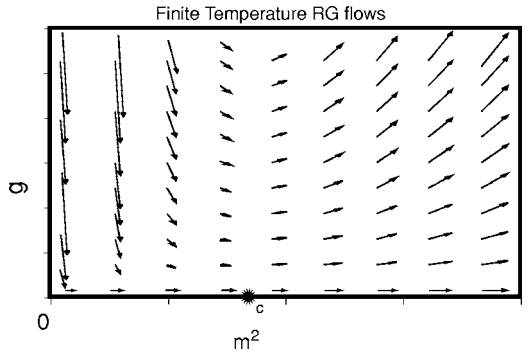

FIG. 5. Renormalization group flows in $\{m^2, g\}$ parameters.

$$\frac{dg}{ds} = \left(\frac{5}{2} - \frac{\Gamma\left[\frac{2}{3}\right]}{8m^2\sqrt{\pi}\gamma^{2/3}}\right)g, \quad (23)$$

$$\frac{d(m^2)}{ds} = \frac{1}{2}m^2. \quad (24)$$

The resultant flows in the $\{m^2, g\}$ plane are shown in Fig. 5. The differential RG equations show that m^2 always grows and that the flow of the variable g changes sign from positive to negative as m^2 becomes smaller than

$$\frac{\Gamma\left[\frac{2}{3}\right]}{20\sqrt{\pi}\gamma^{2/3}},$$

indicated by point c on the plot. However this point is of no special importance because there is no phase transition: recalling that $m^2 \sim 1/T$ we see that the temperature always flows to zero. Thus, the system remains in the same phase with flat domain walls that it has at $T=0$, even as the temperature becomes finite. This formal RG result thus confirms the earlier expectation based on Eq. (15). This result is to be contrasted with the first order flow equations for the case of short range interactions where $dm^2/ds=0$ and flows are vertical at this level of approximation, cf. Eq. (2.24) in Ref. 18 truncated to first order in y, with y and J being the analogs of g and m^2, respectively, in our analysis. It is interesting to note that simple tree level RG rescaling in a d-dimensional (short-range) sine-Gordon model yields $dJ/ds=(d-2)J$, in the analogous notation of Ref. 18, suggesting that our model is in effectively $\frac{5}{2}$ dimensions.

In addition to this classical case, we have also considered the quantum mechanical case, which is equivalent to a classical sine-Gordon model in one extra dimension. Since this raises the dimensionality of the system even more, we find that there is no quantum roughening either.

B. Further possibilities: Stepped surfaces

It is also interesting to consider the possibility of steps and investigate whether the steps themselves are smooth or rough. As our system we considered two semi-infinite three-dimensional domains of antiparallel magnetization in the

z-direction and added to the domain interface a unit lattice step in the x-direction. The magnetization vector in this case is defined by a one-dimensional interface height function $h(z)$,

$$\mathbf{M} = \{0,0,m_0\,\mathrm{sgn}(x - a\Theta[y - h(z)])\}. \tag{25}$$

For the case of short-range forces as shown in Fig. 4, the classical interface is always rough. Here we investigate the effect of the long range forces at finite temperatures. A similar problem has been investigated by Thouless[21] who looked at one-dimensional Ising systems that have long range interactions $\sim r^{-2}$. He concluded that for interactions that fall off faster than r^{-2} there cannot be an ordered state, whereas for an interactions that falls off as r^{-2} the order cannot go continuously to zero. Even though our one-dimensional interface problem is a height model, not an Ising model, the Thouless results suggest that the interface may be rough at finite temperatures.

As before we obtain the energy for the step fluctuations in analogy with electrostatics,

$$U_S = 2m_0^2 a^2 \int dz dz' \frac{h'(z)h'(z')}{[(h(z) - h(z'))^2 + (z - z')^2]^{1/2}}. \tag{26}$$

By assuming that $\theta < 1$ we get to zeroth order in $(h(z) - h(z'))$ the step fluctuation energy in Fourier space,

$$U_{S0} = 4\pi m_0^2 a^2 \int \frac{dk_z dk_y}{(2\pi)^2} \frac{k_z^2}{(k_y^2 + k_z^2)^{1/2}} |h(k_z)|^2. \tag{27}$$

Our approximation scheme here introduces the necessity for an ultraviolet cutoff, Λ_y in the k_y integral, which is set by the discreteness of the lattice, and namely, that the two height variables considered in the correlator are not evaluated at arbitrarily close points, but are at the very least on adjacent lattice sites.

If we now consider the mean height correlation, and once more introduce a surface tension term, $\gamma_s k_z^2$, we have,

$$G_s = \langle (h(z) - h(0))^2 \rangle = \int \frac{dk_z}{2\pi} \frac{1 - e^{ik_z z}}{4\beta m_0^2 k_z^2 \ln\left(\frac{\Lambda_y}{|k_z|} + \gamma_s\right)}. \tag{28}$$

In the large distance limit $G_s \sim L/\ln L$, and the Gaussian model is rough at all finite temperatures. The long range interaction gives rise to a logarighmic term in the energy, raising the effective dimensionality of the system only very slightly above one. This suggests that if we were to take into account the lattice structure by adding a periodic pinning potential to form another modified sine-Gordon model there would be no effect on the roughness of the interface since the periodic sine term cannot pin the interface in dimensions lower than 2. This is clear if we keep in mind that the usual sine-Gordon model for short range interactions only displays a phase transition in exactly two dimensions, where the free Gaussian model has logarithmically divergent correlations. In the usual sine-Gordon model in one dimension the sinusoidal pinning potential is unable to control the linearly diverging correlations of the free Gaussian model, and hence interfaces remain rough. This argument suggests that for the long-range sine-Gordon model in one dimension where the effective dimensionality is close to one, the parameters flow to the high temperature limits, and just as for the case of short range forces, the periodic potential is unable to pin the step which fluctuates freely and hence is rough at all finite temperatures.

For the quantum case with short range forces, G_s diverges as $\sim \ln L$ for the Gaussian model and the full sine-Gordon model exhibits a roughening transition in the KT universality class as shown in Fig. 4. Here, for the case of long-range forces in the quantum problem, similar analysis shows that that the divergence of $G_s \sim \sqrt{\ln L}$ is extremely weak for the Gaussian problem, possibly indicating that the sine-Gordon model will be smooth though we have not been able to verify this in a full RG calculation.

IV. DISCUSSION

We have found that even though $LiHoF_4$ interfaces initially appear to be ideal for having a roughening transition, the same long-range interactions which account for the system's domain structure turn out to be also responsible for the lack of a roughening transition. The long-range interaction term which arises from the dipolar interactions effectively raises the dimensionality of the system and makes it equivalent to a sine-Gordon model in dimensions greater than 2. The RG flow diagram, Fig. 5, which we obtain for $m^2 \sim 1/T$ and g, indicates that in effect the roughening transition coincides with the bulk order-disorder transition and the whole ferromagnetic region is smooth. In contrast, a step in the interface seems to have a rough profile at all temperatures, and the long-range interactions do not raise the dimensionality of the step enough to drive it into the smooth phase.

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APPENDIX: RENORMALIZATION DETAILS

In the following we give some more details of the smooth cutoff procedure[18] leading to the differential renormalization group Eqs. (23) and (24). Beginning with our choice for a smooth cutoff function,

$$f(k_y,k_z) = e^{-a^2(k_z^2 + \gamma a|k_y|^3)}, \tag{A1}$$

and using $k_z' = e^{(3/2)s}$, $k_y' = e^s k_y$, we obtain for small s a rescaled cutoff

$$f'(k_y',k_z') = e^{-a^3 e^{-3s}((k_z'^2/a) + \gamma|k_y'|^3)} \tag{A2}$$

$$\approx f(k_y',k_z') + \zeta(k_y',k_z') + O(s^2), \tag{A3}$$

with

$$\zeta(k_y',k_z') = 3sa^3\left(\frac{k_z'^2}{a} + \gamma|k_y'|^3\right)f(k_y',k_z'). \tag{A4}$$

We can now define a new field, say $\chi(\mathbf{r})$, having ζ as its smooth cutoff. We consider a sine-Gordon model for both the χ and ϕ fields and write

$$S' = S_0[\phi',f] + S_1[\chi,\zeta] + S_{01}[\phi',\chi], \tag{A5}$$

with

$$S_0[\phi',f] = -\frac{m^2}{\pi}\int \frac{d^2\mathbf{k}e^{(1/2)s}}{(2\pi)^2 f(k_y,k_z)}\left\{\frac{k_z^2}{a|k_y|} + \gamma(k_y^2)\right\}|\phi'(\mathbf{k})|^2, \tag{A6}$$

$$S_1[\chi,\zeta] = -\frac{m^2}{\pi}\int \frac{d^2\mathbf{k}e^{(1/2)s}}{(2\pi)^2 \zeta(k_y,k_z)}\left\{\frac{k_z^2}{a|k_y|} + \gamma(k_y^2)\right\}|\chi(\mathbf{k})|^2, \tag{A7}$$

and

$$S_{01}[\phi',\chi] = \frac{g'}{a^2}\int d^2\mathbf{r}\cos(\phi'(\mathbf{r}) + \chi(\mathbf{r})). \tag{A8}$$

It is straightforward to show[18] that the action S' results in the same partition function corresponding to the rescaled action S in Eq. (18). In Ref. 18 this is done by mapping to the Coulomb gas, but an easier method is simply to shift the argument of the cosine term by $-\chi(\mathbf{r})$ and then carry out the Gaussian integral over $\chi(\mathbf{r})$, to recover the rescaled action S.

Now, as part of the RG calculation we integrate out the extra field χ to restore the original cutoff function. We use a cumulant expansion, in S_{01} and write

$$Z = \int D\phi' e^{S_0}\langle e^{S_{01}}\rangle_1 = \int D\phi' e^{S_0} e^{\langle S_{01}\rangle_1 + (1/2)[\langle S_{01}^2\rangle_1 - \langle S_{01}\rangle_1^2] + O(S_{01}^3)}, \tag{A9}$$

where the averaging $\langle\ \rangle_1$ indicates integrating out the extra $\chi(\mathbf{r})$ fields using the Gaussian action S_1. In addition, a multiplicative constant has been absorbed into the measure.

In this analysis we consider the first term in the exponential of the cumulant expansion

$$\langle S_{01}\rangle_1 = \left\langle \int d^2\mathbf{r}\left(\frac{g'}{a^2}\right)\cos(\phi'(\mathbf{r}) + \chi(\mathbf{r}))\right\rangle_1$$
$$= \int d^2\mathbf{r}\left(\frac{g'}{a^2}\right)\cos(\phi'(\mathbf{r}))\langle\cos(\chi(\mathbf{r}))\rangle_1$$
$$- \sin(\phi'(\mathbf{r}))\langle\sin(\chi(\mathbf{r}))\rangle_1. \tag{A10}$$

The average over the sine term is zero by symmetry. For the other term we can use the result for Gaussian integrals which states

$$\langle e^{-i\phi(\mathbf{r})}\rangle_{\text{Gaussian}} = e^{-(1/2)\langle\phi(\mathbf{r})^2\rangle_{\text{Gaussian}}}, \tag{A11}$$

so we obtain

$$\langle S_{01}\rangle_1 = \int d^2\mathbf{r}\left(\frac{g'}{a^2}\right)\cos\phi'(\mathbf{r})\langle\cos(\chi(\mathbf{r}))\rangle_1$$
$$= \int d^2\mathbf{r}\left(\frac{g'}{a^2}\right)\cos\phi'(\mathbf{r})e^{-(1/2)\langle\chi(\mathbf{r})^2\rangle_1}. \tag{A12}$$

The average of $\chi(\mathbf{r})^2$ is given by

$$\langle\chi(\mathbf{r})^2\rangle_1 = \int \frac{d^2\mathbf{k}}{(2\pi)^2}\frac{a\pi|k_y|e^{-(1/2)s}\zeta(k_y,k_z)}{2m^2\{k_z^2 + \gamma a|k_y|^3\}} = \frac{se^{-(s/2)}\Gamma\left[\frac{2}{3}\right]}{4m^2\sqrt{\pi}\gamma^{2/3}}. \tag{A13}$$

We gather our results to obtain

$$\langle S_{01}\rangle_1 = \int d^2\mathbf{r}\left(\frac{g'}{a^2}\right)\cos\phi'(\mathbf{r})e^{-[se^{-(s/2)}\Gamma[2/3]]/[8m^2\sqrt{\pi}\gamma^{2/3}\}}$$
$$\approx \left(\frac{g_s}{a^2}\right)\int d^2\mathbf{r}\cos\phi'(\mathbf{r}) + O(s^2), \tag{A14}$$

where we have introduced the renormalized coupling g_s, which is related to the original g coupling,

$$g_s = \left(1 - \frac{s\Gamma\left[\frac{2}{3}\right]}{8m^2\sqrt{\pi}\gamma^{2/3}}\right)g' \approx \left(1 + \left(\frac{5}{2} - \frac{\Gamma\left[\frac{2}{3}\right]}{8m^2\sqrt{\pi}\gamma^{2/3}}\right)s\right)g. \tag{A15}$$

From the above relation we obtain the differential renormalization Eq. (23). Note that m^2 receives no further corrections to this order in the cumulant expansion and hence Eq. (24) is obtained directly from Eq. (20).

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