RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 32, NUMBER 5 1 SEPTEMBER 1985

Critical dynamics, Lifshitz tricriticality, and supersymmetry: The Ising model on the hcp lattice

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(Received 22 February 1985)

Critical dynamics in d dimensions can be mapped onto a supersymmetric equilibrium problem in $d+1$ with a Lifshitz tricritical point. The existence of such a point is demonstrated for the Ising model on the hcp lattice by Monte Carlo simulation.

Mapping the dynamic properties of models in d dimensions onto the static equilibrium properties of related models in $d+1$ dimensions is often an informative procedure. One way to establish such a mapping proceeds by relating the (continuous-time) dynamics to a quantum Hamiltonian in d dimensions which commutes with the transfer matrix of some $(d+1)$-dimensional classical model.[1,2] Alternatively, one can map the discrete-time Glauber dynamics of a d-dimensional classical problem onto the statics of a $(d+1)$-dimensional one.[3,4]

Through this type of mapping, the dynamical critical properties of the exactly solvable Ising model on a honeycomb lattice were used to predict some critical properties of the so-far unsolvable Ising model on a hcp lattice.[4] These properties were predicted along a line

$$\exp(4J)=\cosh D/\cosh(3D) \tag{1}$$

parametrized by J and D, the temperature-reduced, nearest-neighbor, in-plane ($\parallel$), and out-of-plane ($\perp$) coupling constants for the Ising model. It was also shown[4] that along (1) a transition from a paramagnetic ($D<D_c$) to a ferromagnetic phase exists, where $D_c=\frac{1}{2}\ln(2+\sqrt{3})$ is the critical value of the coupling constant for the Ising model on a honeycomb lattice.

The mapping, however, also predicted several surprising properties for the hcp lattice: along (1), even at the transition point (J_c,D_c), where $J_c=J(D_c)$, the free energy is analytic, and at this transition between two spatially homogeneous phases the static, spatial correlations are anisotropic with correlation lengths $\xi_\parallel\sim|D-D_c|^{-\nu}$ and $\xi_\perp\sim|D-D_c|^{-z\nu}$, where $\nu=1$ and z equals the dynamic exponent of the two-dimensional (2D) problem. The anisotropy is easily understood if the transition point is identified[2,4] as a Lifshitz point[5] of the 3D problem with $m=2$ soft directions. At such a point three lines of transitions meet: the paramagnetic (P) to ferromagnetic (F), P to modulated (M), and M to F lines. The modulated phase is characterized by a wave vector $k_\parallel^M$, and on the P-M transition line $k_\parallel^M\rightarrow 0$ as the Lifshitz point is approached. In this picture, the special line (1) corresponds to a trajectory in the (J,D) plane of the hcp Ising model that lies in the P phase (for $D<D_c$), passes through the Lifshitz point at (J_c,D_c) and either continues into the F phase (for $D>D_c$) or serves as its boundary. At such a point anisotropic scaling is expected. However, when the claim that the dynamic-static problem in d (spatial) dimensions is equivalent to the standard Lifshitz problem in $d+1$ dimensions is scrutinized, several apparent inconsistencies are encountered.

First, the *classical* result for the dynamic-static problem[6] is $\nu_\parallel^c=\frac{1}{2}$, $\nu_\perp^c=z\nu_\parallel^c=1$. For the Lifshitz problem, however, $\nu_\parallel^c=\frac{1}{4}$, $\nu_\perp^c=\frac{1}{2}$; that is, the exponents are off by a factor of 2 and only their ratio, $z=2$, is the same in the classical limits of the two problems. A *second* and more serious inconsistency concerns the upper critical dimension, below which exponents deviate from their classical values. For the static-dynamic problem this is $d_u=4$, while for a Lifshitz point with $m=d$ "soft" directions

$$d_u^L=d_u+1=4+m/2=4+d_u/2\ , \tag{2}$$

yielding $d_u=6$. *Third*,[4] even though the system undergoes a phase transition, the free energy is analytic along line (1).

In this Rapid Communication we offer a resolution of these inconsistencies by identifying the transition point as a Lifshitz tricritical point and substantiate this claim with Monte Carlo simulations of the Ising model on a hcp lattice. We first motivate the claim by considering the mapping for the ϕ^4 field theory in the continuum limit and at the same time show that the resulting Hamiltonian in $d+1$ dimensions is supersymmetric, which accounts for the analyticity of the free energy.

We start by noting that for a d-dimensional model characterized by a Hamiltonian density $\mathscr{H}[\phi(x)]$ the Langevin equation for the time evolution of the field $\phi(x,t)$ is

$$\frac{\partial\phi}{\partial t}=-\frac{\delta\mathscr{H}}{\delta\phi}+\zeta\ , \tag{3}$$

where $\zeta(x,t)$ is a random Gaussian noise, described by the probability

$$P_G[\zeta(x,t)]\sim\exp\left[-\frac{1}{2\sigma}\int d^dx dt\,\zeta^2(x,t)\right]\ , \tag{4}$$

with $\sigma=2k_BT$. Changing variables and expressing the probability of observing a space-time history of the ϕ field[7-9] as

$$P[\phi(x,t)]=P_G\{\zeta[\phi]\}\left\|\frac{D\zeta}{D\phi}\right\|\ , \tag{5}$$

we find from (3) that

$$P[\phi] \sim \exp\left\{ -\frac{1}{2\sigma} \int d^d x dt \left[\left(\frac{\partial \phi}{\partial t} + \frac{\delta \mathscr{H}}{\delta \phi} \right)^2 + \mathscr{H}_J \right] \right\} , \quad (6)$$

where $\exp(-\mathscr{H}_J/2\sigma)$ represents the (formally) exponentiated form of the Jacobian $||D\zeta/D\phi||$. Obviously, since $\phi(x,t)$ appears in the dynamic process with probability $P[\phi]$ and the latter can be viewed as

$$\exp\left[-\int d^{d+1}y \mathscr{H}_{\text{eff}}[\phi(y)] \right] ,$$

we have mapped the dynamic problem in d dimensions onto an equilibrium problem in $d+1$, with $y_{\parallel} = x$ (d components) and $y_{\perp} = t$. Derivations of $\mathscr{H}_{\text{eff}}$ in this manner appear in the literature in various forms.[7-9] Often $||D\zeta/D\phi||$ is expressed[8,9] as a functional integral over fermionic variables ψ, leading to a supersymmetric $\mathscr{H}_{\text{eff}}[\phi,\psi]$. However, if the continuum limit in time is taken for a spatially discrete lattice, the integration over the fermionic variables can be carried out, and one finds $-(1/2\sigma)\mathscr{H}_J = \frac{1}{2}(\delta^2\mathscr{H}/\delta\phi^2)$. Furthermore, since $\mathscr{H}_{\text{eff}}$ is supersymmetric, its lowest eigenvalue is zero,[10] and the free energy of models defined in this manner, such as the hcp Ising model on the line (1), is analytic.

Concentrating in (6) on the term $(\partial\phi/\partial y_{\perp} + \delta\mathscr{H}/\delta\phi)^2$, we note that the cross term is a complete time derivative, and as such yields to $\int d^{d+1}y \mathscr{H}_{\text{eff}}$ a surface term with no bulk contribution to the free energy.

Considering now critical dynamics of the d-dimensional Hamiltonian

$$\frac{1}{k_B T}\mathscr{H} = \frac{1}{2}[r\phi^2 + (\nabla_{\parallel}\phi)^2] + u\phi^4 , \quad (7)$$

we obtain using (7) in (6), an $\mathscr{H}_{\text{eff}}$ in $d+1$ dimensions of the form

$$\mathscr{H}_{\text{eff}} = \frac{1}{2}[R\phi^2 + \mu(\nabla_{\parallel}\phi)^2 + (\nabla_{\parallel}^2\phi)^2 + (\nabla_{\perp}\phi)^2] + v\phi^3\nabla_{\parallel}^2\phi + U\phi^4 + w\phi^6 + \mathscr{H}_J , \quad (8)$$

with $R \sim r^2$, $\mu \sim r$, and $U \sim r$. For the moment disregarding $\mathscr{H}_J$ and shifts caused by fluctuations, we see that the $r=0$ critical point of the d-dimensional model corresponds to a Lifshitz tricritical (LTC) point with $R=\mu=U=0$ in $d+1$ dimensions, and that *two* terms, ϕ^6 and $\phi^3\nabla_{\parallel}^2\phi$, destabilize the classical (e.g., Gaussian) LTC fixed point. These destabilizing terms become relevant for $d^L = d+1 < 5$, that is, when $d < d_u = 4$. This agrees with the upper critical dimension of the static-dynamic problem, thereby resolving one of the inconsistencies. The term $\mathscr{H}_J$ can shift bare couplings from their classical LTC values, but this appears to be[11] precisely the shift needed to account for the effect of fluctuations, at least to order $\epsilon = 4-d$. For $d > d_u$ fluctuations can be neglected, and the behavior is that of a Gaussian LTC model with $R=r^2$, which accounts for factor of 2 inconsistency between the classical values of the exponents.

We now report on the first stage of standard Monte Carlo simulations of the Ising model on the hcp lattice aimed at substantiating the claims made above, namely, that (J_c, D_c) is a LTC point. Our findings do support this claim. The phase diagram, obtained from simulations with $2\times10^3 - 10^4$ spins with 10^4 Monte Carlo steps per spin, is shown on Fig. 1. Three phases are clearly identified: paramagnetic (P), ferromagnetic (F), and an ordered, possibly commensurate phase (O). The special line (1) indeed lies in the paramagnetic phase for $D < D_c$. For $D > D_c$ it is very close to the boundary of the F phase, and probably coincides with it. A continuous transition line from P to F, of (3D) Ising character, passes between the critical point of the $d=2$ Ising model on the triangular lattice, $(J_{\Delta}, 0)$, and the LTC point. However, the P-F transition becomes first order for $D > D_c$, as seen in a jump in the magnetization, and in a double-peak structure of the energy histograms (see Fig. 2). These observations confirm the tricritical nature of the special transition point.[12] To confirm its Lifshitz nature, we calculated the structure factor $\hat{G}(\mathbf{k}) = \langle S(\mathbf{k})S(-\mathbf{k})\rangle$, where $S(\mathbf{k})$ is the Fourier transform of the Ising spins. Our observations indicate that the paramagnetic phase extends to low temperatures, way beyond the LTC point. Thus, the modulated phase (expected classically) seems to be washed out by the strong fluctuations.

In the paramagnetic phase we identify a Lifshitz line:[5] to

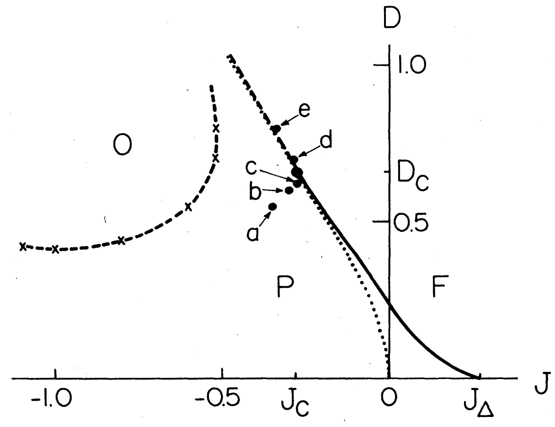

FIG. 1. Phase diagram of the Ising model on the hcp lattice. $J(D)$ are the in-plane (out-of-plane) couplings divided by $k_B T$. The ferromagnetic phase (F) can be reached from the paramagnetic (P) phase by a continuous transition (solid line) or a first-order one (dashed line). The heavy dot at (J_c, D_c) is the Lifshitz tricritical point. The ordered phase (O) is separated from P by a first-order line. Points a–e indicate where the data of Figs. 2 and 3 were collected. The dotted line corresponds to Eq. (1).

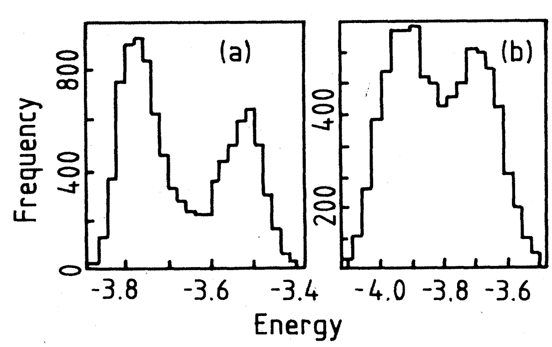

FIG. 2. Energy histograms taken at (a) $J=-0.3464$, $D=0.8$ (point e on Fig. 1) and (b) $J=-0.2892$, $D=0.7$ (point d on Fig. 1). No double peak is seen for $D < D_c$.

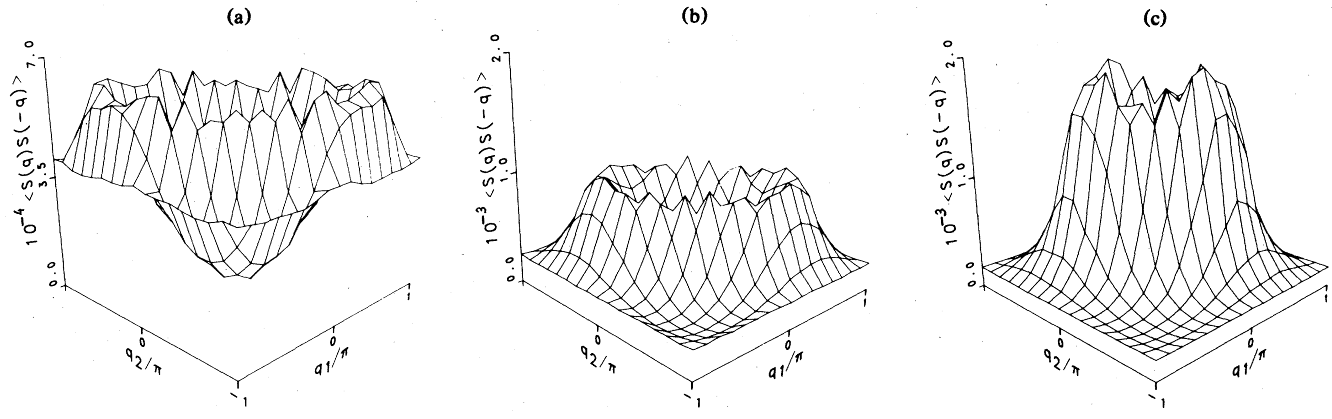

FIG. 3. Structure factor $\hat{G}(\mathbf{q})$ (taken at points a,b,c on Fig. 1). The maxima form a ring that shrinks towards $\mathbf{q}=0$ as the LTC point is approached.

its left, $G(\mathbf{k})$ has a ring of maxima, centered around $\mathbf{k}=0$. As the Lifshitz line is approached, the ring shrinks (see Fig. 3), towards $\mathbf{k}=0$; a single peak is found on the line and to its right. The Lifshitz line lies between (1) and the P-F transition line. These lines meet at the special transition point (J_c,D_c). Similar small deviation of the Lifshitz line from the disorder line was observed in a two-dimensional model.[13] In our case (1) cannot be called a disorder line, since the system orders on it for $D > D_c$.

These observations clearly indicate the Lifshitz nature of the special transition point, and therefore the claim of it being a Lifshitz tricritical point is most strongly supported by our numerical findings. We have also found anisotropic scaling of the specific heat at $(J_c D_c)$, for system sizes ranging from 10^3 to 30^3, again confirming the Lifshitz nature of the multicritical point.[14]

A number of points have not been addressed in detail. One is to determine whether or not the paramagnetic phase extends all the way to $T=0$. So far we concentrated on temperatures close to the LTC point, and we can only say with certainty that the paramagnetic phase becomes narrower as T decreases. Another concerns the nature of the phase denoted by O. Arguments[15] similar to those used for the fcc antiferromagnet[16] suggest that at a sufficiently low temperature a commensurate phase with $\mathbf{k}_\parallel = (\frac{1}{2},0)$ should exist. This structure consists of identical xy planes that have straight rows of spins of alternating sign. Instead of straight rows, we observe kinky lines, corresponding to various degenerate ground states of the hcp lattice. Whether these states with kinks constitute a genuine thermodynamic phase that undergoes a transition to the $(\frac{1}{2},0)$ phase at low temperature, or defects that should disappear with sufficient annealing, is unresolved. Along the line $D=J$ our system is equivalent to the standard hcp Ising antiferromagnet. This, in turn, is closely related to the fcc antiferromagnet;[16] indeed we find that the transition temperatures for both systems are very close: $-J/k_B T \simeq 0.56$. A third issue for future study is the possible existence of a modulated phase with algebraic decay of correlations.

In summary, we found strong numerical support of the claim that the Ising model on the hcp lattice has a Lifshitz tricritical point. As has been shown, the critical dynamics of the $d=2$ Ising model correspond to static critical behavior on a special line that goes through the LTC point. The part of this special line that lies in the paramagnetic phase is close to the Lifshitz line. The low-temperature part of the special line is very close to the first-order boundary of the ferromagnetic phase. The fact that a two-parameter model contains a LTC point (for which in general three parameters must be properly tuned) is probably due to some "hidden" symmetry of the hcp Ising model that reflects the supersymmetry of the continuum model discussed above. We note that a physical system with a LTC point, with $m=2$ "soft" directions, will provide a direct experimental realization of supersymmetry.

We thank B. Halperin for a most illuminating discussion, and A. Aharony, M. E. Fisher, J. Lebowitz, and T. Schneider for calling various references to our attention and for useful comments. J.G. acknowledges the support of the U.S. Department of Energy and E.D. thanks Los Alamos National Laboratory for the hospitality extended to him.

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