# Fully and partially frustrated simple-cubic Ising models: Landau-Ginzburg-Wilson theory

Daniel Blankschtein, M. Ma, and A. Nihat Berker
*Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139*
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Ising models are studied, with frustration covering either only the $x$-$y$ planes, or all the planes of a simple-cubic lattice. The former reveals a two-component ($XY$) order parameter subject to eightfold symmetry breaking. The latter has a four-component Hamiltonian with two fourth-order invariants. Renormalization-group analysis using $d=4-\epsilon$ expansion indicates, respectively, $XY$ criticality and, to order $\epsilon^2$, a first-order transition. Two connected networks, one ordered and one disordered, can form in the fully frustrated system.

Ising spin systems with randomly distributed ferromagnetic ($J$) and antiferromagnetic ($-J$) nearest-neighbor interactions are simple and important examples of spin glasses.[1] In such systems, intrinsic and removable randomness have been distinguished.[2] The latter type can be eliminated by local redefinitions of spin directions and, hence, does not affect the critical properties.[3] Intrinsic randomness has been associated with frustration:[2] The individual local interaction energies cannot all be simultaneously minimized. The total energy is minimized equally by a large number of spin configurations, characterized by the interactions that are violated. On a cubic lattice, each elementary square composed of one and three bonds of opposite signs (and equal magnitude) is frustrated. Frustration is expected to affect strongly the cooperative behavior of a system.

Highly frustrated, but nonrandom systems have been studied as problems related to spin glasses.[4–10] The fully frustrated Ising model on the square lattice is solved exactly[4,5] and remains paramagnetic at all nonzero temperatures. A critical point occurs at zero temperature, where the correlation function decays with a power law. The ground state is highly degenerate, and the entropy per spin is finite at zero temperature. It is of importance to generalize this model to three dimensions, since, due to the higher connectivity, a finite-temperature ordering of a highly degenerate system appears possible.

Consider the fully frustrated Ising model on the square lattice. Figure 1(a) shows the "comb" representation of this model, which is equivalent, via redefinitions of spin directions, to the model originally introduced by Villain.[4] One generalization to three dimensions ($d=3$) is to stack $d=2$ models and to connect them by ferromagnetic nearest-neighbor bonds along the $z$ direction.[10] In this case, only the $x$-$y$ planes are (fully) frustrated [Fig. 1(b)]. Another generalization is to proceed as before, but with every other $d=2$ model shifted by one lattice constant perpendicular to the combs. Every elementary square of this latter system is frustrated [Fig. 1(c)]. In fact, by variously and repeatedly stacking and stagger-stacking, a variety of $d$-dimensional hypercubic lattices frustrated in $\bar{d}$ dimensions, $\bar{d} \leq d$, can be created from the comb model.

Both of these $d=3$ models have highly degenerate ground states, but their entropy per spin vanishes at zero temperature.[6] In the stacked model, at zero temperature, the energy price of introducing a domain boundary along the $z$ direction dominates the concurrent entropy gain,[10] so that one expects long-range order, presumably extending to finite temperatures. A Monte Carlo simulation of the fully frustrated model suggests a finite-temperature phase transition, which appears to be second order.[8]

The construction of a Landau-Ginzburg-Wilson (LGW) Hamiltonian is very profitable in phase transition studies,

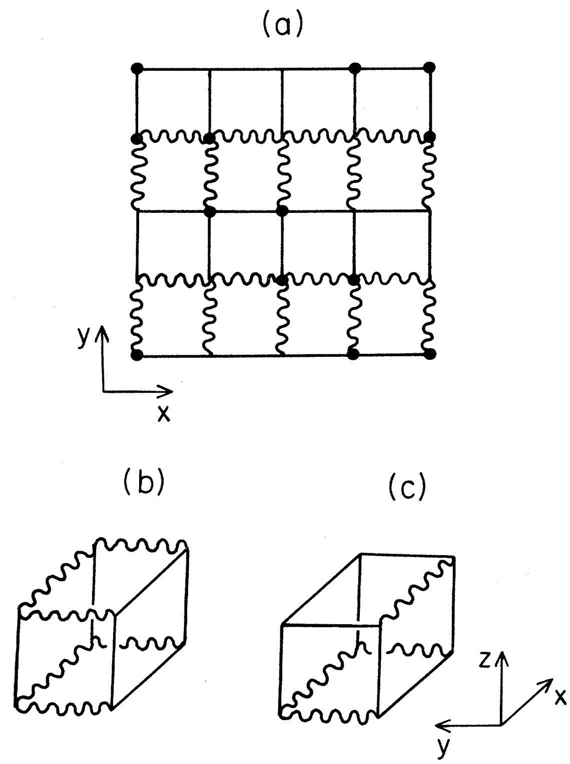


FIG. 1. (a) Comb representation of the fully frustrated square lattice. Straight (squiggly) lines represent ferromagnetic (antiferromagnetic) bonds. A $\pi/2$ rotation has to be combined with spin reversals at the dotted sites to accomplish a symmetry operation. Cubes from the stacked (b) and fully frustrated (c) $d=3$ models.

not only because there are well-developed techniques treating such Hamiltonians, but also because this allows the prediction of critical universality classes[11,7] and of possible onsets of order as demonstrated below. Our present results were made possible by a new application of LGW theory, in which combined usage is made of symmetry operations in position and spin spaces.

The analysis starts with the spin Hamiltonian

$$\mathscr{H}=-\sum_{\langle ij\rangle} J_{ij}s_is_j ,$$

where $s_i=\pm 1$ is the spin at site $i$ of a simple-cubic (SC) lattice, the sum is over nearest-neighbor pairs, and the coupling constant $J$ is periodically ferromagnetic ($J>0$) or antiferromagnetic as specified above and in Fig. 1. The matrix $J_{ij}$ is diagonalized after Fourier transforming. This does not truly solve the many-body problem, since the hard-spin condition $s_i=\pm 1$ translates into a constraint in momentum space $N^{-1}\sum_{\vec{k}} s(\vec{k})s(\vec{q}-\vec{k})=\delta(\vec{q})$. A basic hypothesis is that this constraint is not conserved under rescaling and therefore is irrelevant to asymptotic criticality. Thus it is inferred that the mode(s) with the largest eigenvalue of the interaction matrix becomes critical as temperature is lowered from the disordered phase. The number of critical modes gives the number $n$ of components of the order parameter, which, together with $d$ and the LGW invariants to be discussed below, determine the universality class.

In the stacked model, the Fourier transformed interaction matrix couples modes of wave vectors $\vec{q}$ and $\vec{q}+\pi\hat{y}$ (where $\hat{y}$ is the unit vector in reciprocal space). The largest eigenvalue $(1+\sqrt{2})J$ is associated with two degenerate modes ($n=2$) at momenta $(0,\pi/2,0)$ and $(\pi,\pi/2,0)$. The corresponding eigenvectors give the spatial variations of these critical modes,

$$\phi_1=\cos(\tfrac{1}{2}\pi y-\tfrac{1}{8}\pi)e^{i\pi y} ,$$

$$\phi_2=\sin(\tfrac{1}{2}\pi y-\tfrac{1}{8}\pi)e^{i\pi(x-y)} ,$$

as depicted in Fig. 2(a), with translational invariance along the $z$ direction. From the spatial dependence of these modes, their transformation properties under the symmetry operations of the system are extracted. Then the LGW Hamiltonian is constructed by noting all invariants under the symmetries, at each consecutive order in $\phi_{1,2}$.

Note, however, that the Hamiltonian has a lower symmetry than the underlying Bravais lattice, due to the varying interaction signs. The symmetry of the lattice is restored by invoking local up-down symmetry in spin space, a symmetry of the free energy. For example, a $\pi/2$ rotation about the $z$ axis restores the original system only when accompanied by the spin redefinitions $s_i\to -s_i$ at the dotted sites in Fig. 1(a). Under this combined operation, namely a spatial rotation and selective spin flips, the order parameter transforms as $\phi_{1,2}\to(\phi_1\pm\phi_2)/\sqrt{2}$. Performing the remaining space-group operations of the sc lattice with the appropriate spin flips, the LGW Hamiltonian is determined as

$$\overline{\mathscr{H}}=\tfrac{1}{2}\sum_{\vec{q}}(r+q^2)[\psi_1^2(\vec{q})+\psi_2^2(\vec{q})]+\sum_4 u_4[\psi^2]^2 + \sum_6 u_6[\psi^2]^3+\sum_8 \{u_8[\psi^2]^4+v_8\psi_1^2\psi_2^2(\psi_1^2-\psi_2^2)^2\} ,$$

where $\psi_i$ are modes nearby $\phi_i$, the sums $\sum_p$ are over $p$ conserved momenta, and $[\psi^2]\equiv\psi_1^2+\psi_2^2$. The eight-order term takes a more transparent form with the substitution $\psi_1=m\sin\theta$ and $\psi_2=m\cos\theta$, namely, $\sum\{(u_8+v_8/32)m^8-(v_8/32)m^8\cos(8\theta)\}$. Thus the LGW Hamiltonian of the stacked model is that of an $XY$ ($n=2$)

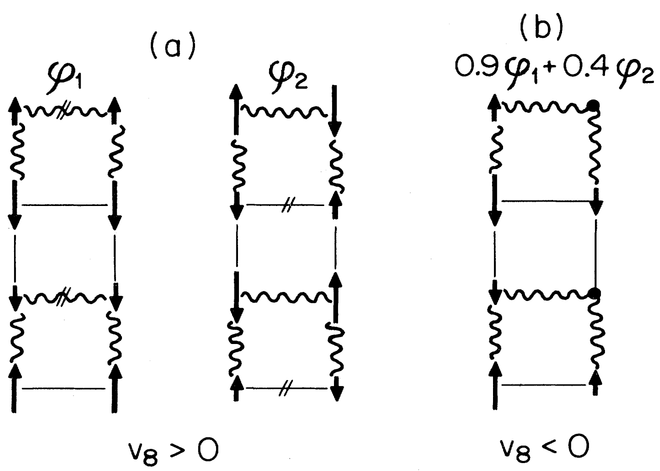


FIG. 2. (a) Eigenmodes of the stacked model. Long and short arrows represent magnitudes of $M\cos(\pi/8)$ and $M\sin(\pi/8)$. These are also, for $v_8>0$, two of the eight degenerate ordered phases. Violated bonds are slashed. (b) Ordered phase for $v_8<0$. Long and short arrows represent magnitudes of $M$ and $M/\sqrt{2}$. Sites without arrows are totally disordered.

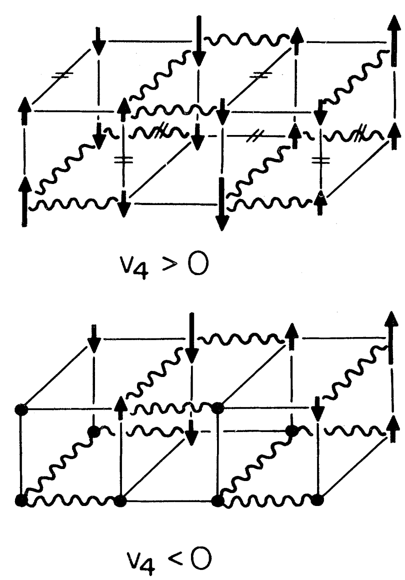


FIG. 3. One of the sixteen degenerate ordered phases of the fully frustrated model, for either sign of $v_4$. Long and short arrows represent magnitudes of $(3-\sqrt{3})^{1/2}M$ and $(3-\sqrt{3})^{1/2}M/\sqrt{3}$ for $v_4>0$, $\sqrt{2}(3-\sqrt{3})^{1/2}M$ and $\sqrt{2}(3-\sqrt{3})^{1/2}M/\sqrt{3}$ for $v_4<0$. Sites without arrows are totally disordered. Violated bonds are slashed. Note the interpenetrating ordered and disordered networks for $v_4<0$.

model with eightfold symmetry breaking. Momentum-space renormalization-group analysis to first order in $\epsilon=4-d$ indicates that $v_8$ is irrelevant at $d=3$. Accordingly, $XY$ criticality is expected, for example, with a cusped ($\alpha \simeq -0.02$) specific heat.[12]

The configuration of the ordered phases just below the transition is given by $M[\phi_1 \sin\Phi + \phi_2 \cos\Phi]$, where $(M,\Phi)=(m,\theta)$ minimize the LGW Hamiltonian. There are eight degenerate phases. For $v_8>0$, $\Phi=0,\pi/4,2\pi/4$, etc. Each critical mode corresponds to an ordered configuration, which is characterized by the interactions of every other row being violated, and the smaller of two average-spin magnitudes $[\sim\sin(\pi/8),\cos(\pi/8)]$ occurring on this row [Fig. 2(a)]. The remaining six phases are obtained by interchanging the roles of rows and columns, and by global spin reversals. For $v_8<0$, $\Phi=\pi/8$, $3\pi/8$, $5\pi/8$, etc. The critical modes are mixed in the ordered configurations [Fig. 2(b)]. In an elementary square, $\pm M$ and 0 occur diagonally; the other diagonal has magnitude $M/\sqrt{2}$, with signs chosen to satisfy bonds with $\pm M$. Thus some linear arrays of spins along the $z$ direction remain totally disordered inside the ordered phase.[4,10] One guesses that $v_8<0$ in the LGW Hamiltonian, since the corresponding phases have a higher entropy, as estimated by $S\sim\sum_i(1-|\langle s_i\rangle/\langle s\rangle_{\max}|)\ln 2$.

The fully frustrated model in $d=3$ is treated similarly. Upon Fourier transforming, the interaction matrix decomposes into $2\times2$ blocks which couple modes of wave vector $\vec{q}$ and $\vec{q}+\pi\hat{y}+\pi\hat{z}$. Diagonalizing these blocks, we find that the largest eigenvalue, $\sqrt{3}J$, is associated with four degenerate modes ($n=4$). The spatial variations of the four components of the order parameter are

$$\phi_1=[\cos(\tfrac{1}{2}\pi y)+A\cos(\tfrac{1}{2}\pi y+\tfrac{1}{4}\pi)e^{i\pi z}]\ ,$$

$$\phi_2=[\sin(\tfrac{1}{2}\pi y)-A\sin(\tfrac{1}{2}\pi y+\tfrac{1}{4}\pi)e^{i\pi z}]\ ,$$

$$\phi_3=[\cos(\tfrac{1}{2}\pi y)-A\sin(\tfrac{1}{2}\pi y+\tfrac{1}{4}\pi)e^{i\pi z}]e^{i\pi x}\ ,$$

and

$$\phi_4=[\sin(\tfrac{1}{2}\pi y)-A\cos(\tfrac{1}{2}\pi y+\tfrac{1}{4}\pi)e^{i\pi z}]e^{i\pi x}\ ,$$

where $A=(\sqrt{3}-1)/\sqrt{2}$. Again the symmetry operations involve combining the space-group operations of the sc lattice and local spin redefinitions. The LGW Hamiltonian, invariant under these operations, is

$$\overline{\mathscr{H}}=\tfrac{1}{2}\sum_{\vec{q}}(r+q^2)\sum_{i=1}^{4}\psi_i^2(\vec{q})+u_4\sum_4\left[\sum_{i=1}^{4}\psi_i^2\right]^2+v_4\sum_4\left[\sum_{i=1}^{4}\psi_i^4-\sqrt{3}(\psi_1^2-\psi_2^2-\psi_3^2+\psi_4^2)(\psi_1\psi_2+\psi_3\psi_4)+3(\psi_1\psi_3+\psi_2\psi_4)^2\right]\ .$$

We have subjected this Hamiltonian to momentum-space renormalization group to second order in $\epsilon=4-d$. There are two fixed points: the unstable Gaussian fixed point ($u_4=v_4=0$) and the isotropic "Heisenberg" fixed point ($u_4\neq v_4=0$), which is marginal to order $\epsilon$, but unstable to order $\epsilon^2$. The interpretation of such renormalization-group runaway flows is a first-order phase transition.[13]

Hypothesizing that this is a weakly first-order transition, consistently with marginality to order $\epsilon$ (also recall the second-order interpretation of Monte Carlo[8]), the configuration of the ordered phases just below the transition is given by

$$M[\phi_1\sin\Phi_1\sin\Phi_2-\phi_2\sin\Phi_1\cos\Phi_2-\phi_3\cos\Phi_1\sin\Phi_3+\phi_4\cos\Phi_1\cos\Phi_3]\ ,$$

$$\Phi_1=\tan^{-1}[2-(\mathrm{sgn}v_4)\sqrt{3}\sigma_1]^{1/2}\ ,$$

$$\Phi_2=[3\sigma_1+6\sigma_2+12\sigma_3+1]\pi/24\ ,$$

$$\Phi_3=[3\sigma_1-(\mathrm{sgn}v_4)6\sigma_2+12\sigma_4-1]\pi/24,\quad \sigma_i=\pm1\ .$$

Thus there are sixteen degenerate phases that are related by up-down symmetry and corner-cubic (face-hypercubic) symmetry for $v_4<0$ ($v_4>0$). For $v_4>0$, lines of violated bonds form a $2\times2$ structure for each direction and do not intersect (Fig. 3). The smaller of two average-spin magnitudes $(\sim 1/\sqrt{3},1)$ occurs next to violated bonds. Each elementary cube has $|\langle s_i\rangle|\sim M$ at two diagonally opposite sites, $|\langle s_i\rangle|\sim M/\sqrt{3}$ at the other sites with signs fixed so that three violated bonds do not touch $|\langle s_i\rangle|\sim M$. For $v_4<0$, ordering occurs only in one of two connected networks (Fig. 3). Each elementary cube has one $|\langle s_i\rangle|\sim M$ connected to $|\langle s_i\rangle|\sim M/\sqrt{3}$ via unviolated bonds, and disorder in the diagonally opposite half. This interpenetrating ordered and disordered portions, each percolating with the full dimensionality of the underlying lattice, is a noteworthy microscopic picture.[9] As above, one guesses by entropy consideration that $v_4<0$ in the LGW Hamiltonian.

It is seen from our study that frustration problems, which derive from hard-spin conditions and discrete lattices, can be addressed by continuum LGW theory, provided the lattice and local spin symmetries are combined. Our results show that frustation affects the universality class of the transitions, providing an example of an apparently Ising ($n=1$) Hamiltonian accommodating $n>1$ criticality. Needless to say, our method is applicable to other arrangements of frustrated squares, and a variety of results are obtained. For example, stacked planes in which periodically two out of three consecutive rows of squares are frustrated give $n=1$ criticality. In a real spin glass, local frustration patterns occur randomly. Thus it is tempting to speculate that a system of vector spins with a randomly variable number of components (random $n$) and random orientations is appropriate for the spin-glass transition. This, in turn, should asymptotically reduce to a random-axis model.

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