"Spiraling" Algorithm: Collective Monte Carlo Trial and Self-Determined Boundary Conditions for Incommensurate Spin Systems

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To study incommensurate spin systems, we employ a collective Monte Carlo trial that enables the system to choose its own boundary conditions. The method is tested on a generalization of the 2D fully frustrated triangular lattice of XY spins. Even for small sizes of our model system, the bulk value for the pitch is obtained. Convergence as a function of size is far better than can be obtained with free or periodic boundary conditions. Moreover, this approach yields the temperature dependence of the pitch in the modulated phase. The spiral-to-antiferromagnetic phase transition appears to be continuous and a Lifshitz point occurs at finite temperature.

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Phase transitions in magnetic systems with competing interactions lead to very rich phase diagrams. Experimental realizations are provided by the heavy rare-earth metals: As a result of the competition, one obtains many complex low-temperature structures, including spiral, sinusoidal, and conical orderings [1]. Quite often, the wave vector k describing the structure is incommensurate with the lattice, so that the pitch $\Delta \equiv ka$, where a is the lattice constant, is not a rational integral multiple of 2π. Much experimental data, giving pitch as a function of temperature T, have remained unexplained for over thirty years.

Incommensurability may affect critical properties. Indeed, new universality classes have been predicted for such systems [2–4]. Nevertheless, presently it is not clear that these predictions account for the experimentally determined values of the critical exponents [5]. To supplement the analytic approaches, Monte Carlo simulations have been performed [6, 7]. Reference [6] restricted its consideration to the case of commensurate spirals. In Ref. [7], the pitch of the helimagnet was given commensurate values appropriate to zero temperature, and the system was then studied as a function of temperature. The restriction to commensurate spirals is made in order that the conventional use of fixed, periodic boundary conditions not impose a constraint that does not occur in the thermodynamic limit.

One approach to incommensurate systems would be to employ periodic boundary conditions and attempt to extrapolate to the thermodynamic limit using a scaling approach. However, when a system is incommensurate (or its pitch is unknown, and perhaps even temperature dependent), periodic boundary conditions may serve to introduce "frustration." This increases the energy of the system and, in extreme cases (e.g., a small system for which the bulk solution has two nearly degenerate phases, or a classical linear antiferromagnet with an odd number of spins), can cause the system to choose the wrong phase entirely. Moreover, because for a system of length L the pitch will be an integral multiple of $2\pi/L$, there will be discontinuous changes in the pitch as L is varied. Trying to scale to obtain the correct pitch would involve finding a function with size-dependent oscillations, and would require very large systems to ensure attainment of the correct thermodynamic limit.

A second approach might be a brute force Monte Carlo study where one imposes a fixed but incommensurate pitch on the system and, for a given temperature, computes the free energy as that pitch varies. The correct value of the pitch would be the one that minimizes the free energy. However, the free energy is one of the more difficult quantities for Monte Carlo calculations to determine [8], and for that reason we did not seriously consider such a calculation.

A third approach, which preliminary calculations indicate to be more practical than either of the above two approaches, is to employ free boundary conditions. However, even in this case one must employ very large sample sizes to eliminate surface effects.

To circumvent the difficulties of these three approaches, *we have developed a "spiraling" algorithm that, employing a collective Monte Carlo trial, allows the system to choose its own boundary conditions. It yields the pitch Δ both for small systems and at finite temperatures.*

We illustrate the spiraling algorithm with the following example. Consider a linear system of three XY spins, 3-4-5, which may be subject to both nearest- and next-nearest-neighbor interactions. It is well known that such a J_1-J_2 model can lead to a spiral state. As a start, one can choose an arbitrary pitch Δ (say, 20°) and small random deviations of each spin from that pitch. One adds two phantom spins to the left and right (the number of phantom spins is determined by the range of the interactions—for nearest-neighbor interactions only, one needs to add only one phantom spin to each side). Spins 6 and 7 are obtained from 3 and 4, respectively, by rotating 3 and 4 clockwise by 3 times 20°. Spins 1 and 2 are

obtained from 4 and 5, respectively, by rotating 4 and 5 counterclockwise by 3 times 20°.

The usual Monte Carlo changes for each spin are then attempted, the change in energy is determined by the above rule for obtaining the new state (if 3 is rotated clockwise by an additional 10°, so is its phantom, 6), and then the new state is tested for acceptance with the Metropolis *et al.* algorithm. *The next step permits the system to choose its own boundary conditions, by attempting to change the pitch* Δ. Such a trial change might be a $\delta\Delta$ of 5°. Then, (arbitrarily) leaving spin 1 unaffected, one rotates the other spins clockwise by an angle that is 5° times their distance from spin 1. This new configuration is then tested for acceptance with the Metropolis *et al.* algorithm. At zero temperature, this procedure finds the appropriate pitch for the spiral and, for $J_2 = 0$ and $J_1 < 0$ (antiferromagnet), the antiperiodic boundary condition (in the present case, a pitch of 180° per spin) appropriate to three spins.

To test the procedure on a nontrivial spiral structure, we have considered the "row" generalization of the 2D fully frustrated triangular lattice of XY spins. Here each spin $\mathbf{S}_i$ has nearest-neighbor interactions only: In $\mathcal{H} = -\sum_{ij} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j$, the two horizontal bonds have $J_{ij} = -\eta J$, and the other four bonds have $J_{ij} = -J$ [9, 10]. [For a typical spin configuration, see Fig. 4 of Ref. [9] or Fig. 1(b) of Ref. [10].] We determine the pitch Δ_1 of the structure at low temperature for $\eta > 0.5$, where it should approach the value given by mean-field theory [9, 10]

$$2\eta \cos(\Delta_1/2) = -1. \tag{1}$$

Thus, at low temperatures, if $\eta = 3$ one expects a pitch of either 199.2° or 160.8°. Employing the spiraling algorithm to obtain the pitch along the x direction (but with periodic boundary conditions along the y direction), we find that, for $T/J = 0.10$ (and 5000 Monte Carlo steps, in which the first 2000 are discarded) the average value of the pitch is 161.0 for 3-by-3, 161.1 for 6-by-6, 161.2 for 12-by-12, and 161.8 for 24-by-24 systems. The systematics in this may be attributed to the longer equilibration times needed for larger systems. Thus the spiraling algorithm finds the correct pitch. (In these runs, a seed pitch of 0.4 rad was taken, but the spiraling algorithm has also determined the correct pitch with a seed pitch of zero.)

The spiraling algorithm should permit reliable finite-size scaling analyses of critical exponents for incommensurate structures. However, because a knowledge of the phase diagram must precede a study of critical properties, we will concentrate on the nature of the phase diagram. We first summarize the mean-field theory results.

Mean-field theory, for $\eta > 0.5$, gives a spiral (Sp) structure that is typically incommensurate [9, 10]; for $\eta < 0.5$, it gives an antiferromagnetic (AF) structure of ferromagnetic horizontal lines whose moment alternates direction as one moves vertically. Because the pitch of the Sp phase approaches π as $\eta \to 0.5$, the transition to the AF phase at $\eta = 0.5$ is continuous, so the AF-Sp line is second order, in mean-field theory. A Lifshitz point, where the Sp, AF, and paramagnetic (P) phases come together, occurs for $\eta_L = 0.5$, $T_L/J = 1.5$.

Going beyond mean-field theory, one expects fluctuations to alter these results: For XY systems the transitions survive at finite T but the low-temperature phases do not possess long-range order in any continuous order parameter. In addition, frustration alters the symmetry of the system, by mixing in an Ising field associated with spirals of opposite twist, or helicity. For $\eta = 1$, a single transition is obtained, with mixed Ising and XY character [11, 12]. For modulated structures with incommensurate wave vectors, a phase diagram has been proposed that displays this feature, plus the additional property that the Lifshitz point is at $T_L = 0$ [13]. This appears reasonable, since the lower critical dimensionality for a uniaxial Lifshitz point is 2.5; however, the argument applies only for spins with at least three components [14].

We now present results for 48-by-48 systems with 40 000 Monte Carlo steps per spin, the first 16 000 discarded for equilibration purposes, and with statistical sampling every 10 steps. We emphasize that the spiraling algorithm makes the calculations possible: There is no intrinsic dependence on lattice size. Study of a number of correlation functions and susceptibilities yields the phase diagram given in Fig. 1. The general shift to lower transition temperatures is indicated by the Lifshitz point moving to $\eta_L = 0.62 \pm 0.02$, $T_L/J = 0.40 \pm 0.02$. Moreover, the AF-Sp line develops a positive slope, rather than being flat, so that there are now three characteristic ranges for η: $\eta < 0.5$, $0.5 < \eta < \eta_L$, $\eta_L < \eta$. Figure 2 gives the spin stiffnesses ρ_{xx} and ρ_{yy} as a function of temperature, for three values of η within each of these ranges. Figure 3 gives the specific heat C_v. There is no real evidence for a peak in C_v at the Sp-AF transition, although calculations on larger systems might be more revealing. Note that the system should be isotropic for $\eta = \pm 1$; in both cases we find $\rho_{xx} = \rho_{yy}$ to within numerical accuracy. Moreover, $\eta = 1$ gives the established

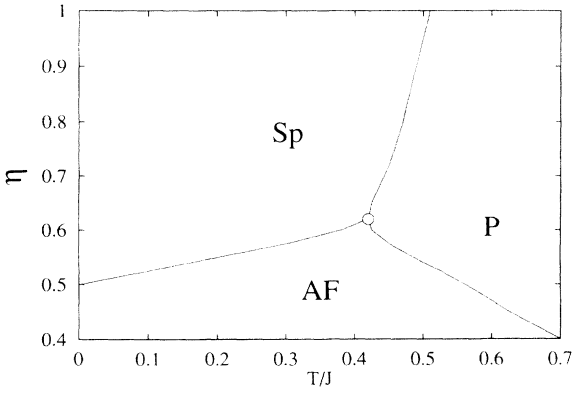

FIG. 1. Monte Carlo phase diagram in the η-T plane.

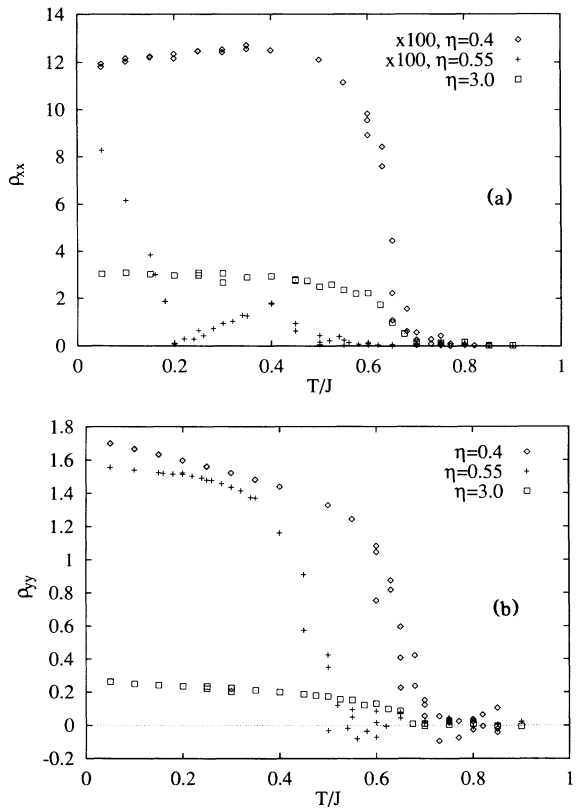

FIG. 2. (a) Spin stiffness ρ_{xx} along the horizontal, as a function of temperature, for characteristic values of the row-exchange parameter η. For $\eta = 0.4$ and $\eta = 0.55$, the values have been multiplied by 100. (b) Spin stiffness ρ_{yy} along the vertical, as a function of temperature, for the same characteristic values of η.

result $T_c/J \approx 0.50$ [11].

When the boundary conditions along the horizontal are permitted to vary, explicit expressions for ρ_{xx}, which assume fixed boundary conditions, are inappropriate [15]. However, when the boundary conditions vary, the fluctuation-defined pitch susceptibility χ_Δ can be employed to determine ρ_{xx}, via

$$\rho_{xx} = 2/\sqrt{3}\chi_\Delta, \qquad \chi_\Delta = \langle(\delta\Delta)^2\rangle/T. \tag{2}$$

($2/\sqrt{3}$ is a geometrical factor relating to the area of the unit cell.) Equation (2) makes it possible, in the AF phase, to determine ρ_{xx} both directly (with fixed boundary conditions) and indirectly (with varying boundary conditions). In particular, the results in Fig. 2 at low T, for $\eta = 0.4$, were obtained using both methods; clearly, the points all lie on the same line. This relation between spin stiffness and the fluctuation in the pitch makes possible the evaluation of the spin stiffness for systems with more than one spin per unit cell, because one then need not know the relative twist between spins within the unit cell (less twist occurs between spins with stiff bonds) [16].

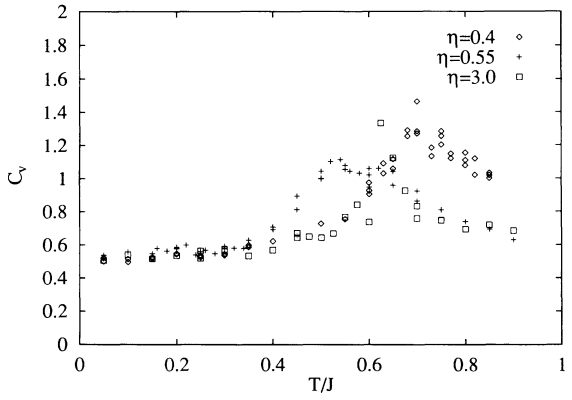

FIG. 3. Specific heat C_v as a function of temperature, for the same values of η as in Fig. 2.

Observe that for $\eta = 0.55$ and $T/J > 0.2$, ρ_{xx} increases on moving away from the Sp-AF phase boundary; such displacement away from the Sp-AF phase boundary also occurs for $\eta = 0.4$ and low temperature, giving the unusual low-temperature increase in ρ_{xx} seen in Fig. 2.

For $\eta = 3$ there is a continuous Sp to P phase transition at $T_c/J = 0.625 \pm 0.025$. For $\eta = 0.55$ there is a continuous Sp to AF phase transition at $T_c/J \approx 0.20$, signaled by a zero in ρ_{xx}, as well as (cf. Fig. 4) by the disappearance of the Ising-like helicity order parameter

$$\psi_{\rm hel} = \frac{1}{3\sqrt{3}N}{\sum_{ij}}'(-1)^{3\Phi_{ij}/\pi}\sin(\theta_i - \theta_j), \tag{3}$$

which is sensitive to the direction of twist of the spiral, and by the appearance of a singularity in its fluctuation-defined susceptibility $\chi_{\rm hel} = \langle(\delta\psi_{\rm hel})^2\rangle/T$. ($\psi_{\rm hel}$ is defined so that it is ± 1 for $\eta = 1$ and $T = 0$. The prime denotes a sum over each of the N sites and their nearest neighbors, and Φ_{ij} is the angle obtained on going from site j to site i, and then rightward, so that $3\Phi_{ij}/\pi = \pm 1$.) There is also a continuous AF to P phase transition at

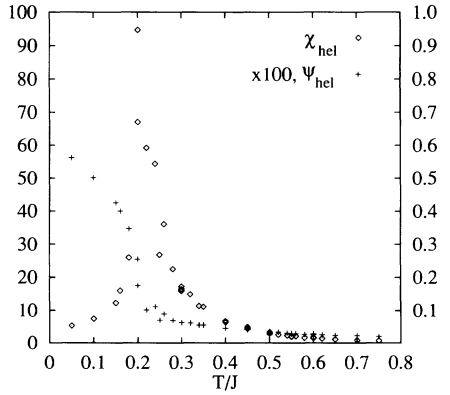

FIG. 4. Helicity $\psi_{\rm hel}$ and its susceptibility $\chi_{\rm hel}$, for $\eta = 0.55$, as a function of temperature. $\psi_{\rm hel}$ is multiplied by 100.

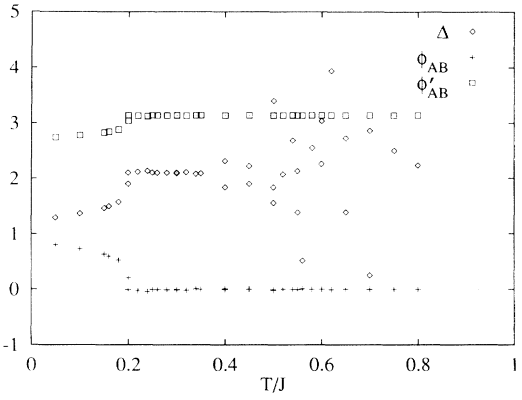

FIG. 5. Monte Carlo pitch Δ, and relative spin orientations with nearest neighbor along the horizontal (ϕ_{AB}) and at 60° (ϕ'_{AB}), for $\eta = 0.55$ as a function of temperature.

$T_c/J \approx 0.50$. For $\eta = 0.4$ there is only a single phase transition from the AF to the P phase. To the accuracy of our calculations, we cannot exclude the possibility of a very narrow strip of P phase (of width $\delta T/J < 0.02$) interposing between the Sp and AF phases, which would then yield $T_L = 0$, such as is found in axial next-nearest-neighbor Ising models [17].

Figure 5 gives Δ and the relative spin orientations for nearest-neighbor vectors along the horizontal (ϕ_{AB}) and at 60° (ϕ'_{AB}). These are computed for $\eta = 0.55$, so that the system passes from Sp to AF to P as T/J increases. Note that $\phi_{AB} + 2\phi'_{AB} \approx 2\pi$ for all three phases. In the Sp phase, the pitch varies with temperature, approaching the pitch of the AF phase as the Sp-AF line is approached; this is consistent with the Sp-AF transition being continuous. This temperature dependence is in contrast to the temperature-independent pitch of Eq. (1), and is to our knowledge the first time a Monte Carlo calculation for XY spins has revealed a temperature-dependent pitch.

We have also considered the "staggered row" model of XY spins on a triangular lattice. This has three spins per unit cell (ABC), only the horizontal A-B bonds being multiplied by η [18]. Its mean-field theory has been studied under the assumption of commensurate states with three spins per unit cell [18]. Application of the spiraling algorithm helped identify three new phases, one of them incommensurate and the other two commensurate with six spins per unit cell [19, 20].

To summarize, we have demonstrated that the spiraling algorithm applied to incommensurate spin systems yields the correct pitch, for both small systems and finite temperatures [21].

[1] See the article by W. C. Koehler, in *Magnetic Properties of Rare Earth Metals*, edited by R. J. Elliot (Plenum, London, 1972).
[2] T. Garel and P. Pfeuty, J. Phys. C **9**, L245 (1976).
[3] P. Bak and D. Mukamel, Phys. Rev. B **13**, 5086 (1976).
[4] H. Kawamura, Phys. Rev. B **38**, 4916 (1988).
[5] See, for instance, J. Wang, D. P. Belanger, and B. D. Gaulin, Phys. Rev. Lett. **66**, 3195 (1991).
[6] H. Kawamura, J. Appl. Phys. **63**, 3086 (1988); (to be published).
[7] H. T. Diep, Phys. Rev. B **39**, 397 (1989).
[8] K. Binder, in *Monte Carlo Methods in Statistical Physics* (Springer-Verlag, Berlin, 1986), 2nd ed.
[9] W. M. Zhang, W. M. Saslow, and M. Gabay, Phys. Rev. B **44**, 5129 (1991).
[10] H. Kawamura, Prog. Theor. Phys. Suppl. **101**, 545 (1990).
[11] D. H. Lee, J. D. Joanopoulos, J. W. Negele, and D. P. Landau, Phys. Rev. B **33**, 450 (1986).
[12] Varying η in a generalized version of the Villain "odd" model [J. Villain, J. Phys. C **10**, 1717 (1977)] dissociates the Ising and XY lines. For Monte Carlo calculations, see B. Berge, H. T. Diep, A. Ghazali, and P. Lallemand, Phys. Rev. B **34**, 3177 (1986); for mean-field theory, see M. Gabay, T. Garel, G. Parker, and W. M. Saslow, Phys. Rev. B **40**, 264 (1989).
[13] T. Garel and S. Doniach, J. Phys. C **13**, L887 (1980).
[14] R. M. Hornreich, M. Luban, and S. Strikman, Phys. Rev. Lett. **35**, 1678 (1975).
[15] For periodic boundary conditions, ρ_{xx} and ρ_{yy} are computed by a generalization of the $\eta = 1$ expression given in Appendix A of Ref. [11]. This result always applied for ρ_{yy} because periodic boundary conditions were always taken along the y direction.
[16] E. Granato and J. M. Kosterlitz, J. Appl. Phys. **54**, 5636 (1988). These authors study the model of Ref. [12]. Its ordered phases have at least two spins per unit cell. To calculate the spin stiffness, the simplifying assumption was made that all spins twist by the same amount.
[17] W. Selke, Phys. Rep. **170**, 213 (1988).
[18] G. Parker, W. M. Saslow, and M. Gabay, Phys. Rev. B **43**, 11 285 (1991).
[19] The results from Ref. [18] can be converted to those for the "centered" honeycomb model, in which *all* the A-B bonds are multiplied by η, if one replaces η by $(2+\eta)/3$.
[20] W.-M. Zhang, W. M. Saslow, and M. Gabay (to be published).
[21] Another view of the "spiraling" algorithm is that it enables one to work within an ensemble of constant "current," rather than one of constant pitch. With ϵ the energy of the system, the current $\partial\epsilon/\partial\Delta$ and the pitch Δ are thermodynamically conjugate variables.