Existence of Phase Transitions for Anisotropic Heisenberg Models

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The two-dimensional anisotropic, nearest-neighbor Heisenberg model on a square lattice, both quantum and classical, has been shown rigorously to have a phase transition in the sense that the spontaneous magnetization is positive at low temperatures. This is so for all anisotropies. An analogous result (staggered polarization) holds for the antiferromagnet in the classical case; in the quantum case it holds if the anisotropy is large enough (depending on the single-site spin).

In statistical mechanics and solid state physics, magnetic systems are often described by models of spins on a cubic lattice with nearest-neighbor quadratic interactions. Moreover, for spin $S=\frac{1}{2}$, these models yield idealized descriptions of hard-core Bose gases. A primary question is whether some of the equilibrium states of such models in the thermodynamic limit have long-range order at low (but nonzero) temperatures, T, i.e., whether there are first-order phase transitions in the magnetic field. To date, the rigorous results for Heisenberg-type models include the following: (i) In three or more dimensions the classical isotropic and anisotropic (ferromagnetic and antiferromagnetic) models have a first-order phase transition.[1] The same is true in the quantum case,[2] except that, for the antiferromagnet, the existence of a phase transition is only known for spin $S\geq 1$. (Here, S is the spin at one site.) (ii) In two dimensions the Ising model (case of extreme anisotropy) has, at low temperatures, equilibrium states with long-range order,[3] but the isotropic Heisenberg ferromagnet or antiferromagnet (including the rotor model) does not.[4] It has been suggested[5] that the two-dimensional isotropic models might have phase transitions not accompanied by long-range order, but this problem will not concern us here.

It is therefore of interest to know whether the two-dimensional anisotropic models have a first-order phase transition, for all anisotropies, i.e., whether they behave more like the Ising model than the isotropic models. An affirmative answer was recently given for the classical ferromagnetic and antiferromagnetic models.[6] Previous work had shown that long-range order exists at low temperatures if the anisotropy is large (in both the quantum[7,8] and classical[9] cases). The open question was whether the quantum fluctuations caused by the xy part of the Hamiltonian could destroy the ordering for small anisotropy.

We have rigorously proved that, at low temperatures, the equilibrium states of the following models have long-range order: the quantum mechanical, ferromagnetic Heisenberg model with arbitrary anisotropy; the quantum mechanical antiferromagnet, provided S is large enough, depending on the anisotropy. As a by-product we have found alternative proofs of the results of Ref. 6.

We consider three different models defined by the Hamiltonians

$$H_p = S^{-2}\{H_p{}^z + \alpha H_p{}^{xy}\}, \quad p=1,2,3,$$

where $0\leq\alpha<1$ is the anisotropy parameter. Model 1 is the usual ferromagnet:

$$H_1{}^z = -\sum S_i{}^z S_j{}^z, \quad H_1{}^{xy} = -\sum\{S_i{}^x S_j{}^x + S_i{}^y S_j{}^y\}$$

(with the sums taken over distinct nearest-neighbor pairs). Model 2 is a more subtle version of model 1:

$$H_2{}^z = \tfrac{1}{2}\sum (S_i{}^z - S_j{}^z)^2,$$

$$H_2{}^{xy} = \tfrac{1}{2}\sum\{(S_i{}^x - S_j{}^x)^2 + (S_i{}^y - S_j{}^y)^2\}.$$

Note that

$$H_2 = H_1 + \frac{1-\alpha}{2S^2}\sum\{(S_i{}^z)^2 + (S_j{}^z)^2\} + C,$$

where C is a trivial constant proportional to $1+ +S^{-1}$. For $S>\frac{1}{2}$, the distinction between H_2 and H_1 is interesting: In the quantum case the ground state of H_1 *and* H_2 is doubly degenerate and has all spins maximally oriented in the z direction. In the classical limit (where the spins become unit vectors and the trace is replaced by integra-

tions over unit spheres[10]) the ground state of H_2 is infinitely degenerate: There is no preferred direction. Thus, in model 2 long-range order is a more subtle phenomenon than in model 1, and this fact causes our estimate for T_c to go to zero as $S \to \infty$, for each fixed $\alpha < 1$, in model 2.[11] In model 1, T_c is bounded away from 0, uniformly in S, for all $\alpha < 1$. Finally, model 3 is the usual antiferromagnet:

$$H_3 = -H_1.$$

To state our theorems we define (for spin S and temperature T)

$$\sigma(S,T) = S^{-2} \lim_{|j|\to\infty} \epsilon_j \langle S_0^z S_j^z \rangle$$

to be the long-range-order parameter for the equilibrium state $\langle\cdot\rangle$ obtained as a thermodynamic limit of Gibbs states $\langle A\rangle_\Lambda = Z_\Lambda^{-1} \mathrm{Tr}[A \exp(-H_p^{(\Lambda)}/kT)]$ with periodic boundary conditions at the boundary of the rectangles Λ. In the ferromagnet $\epsilon_j = 1$, whereas in the antiferromagnet $\epsilon_j = (-1)^{|j|}$.

Model 1: For each $\alpha < 1$ there is a $T_c > 0$ and a function $\mu(T)$, both independent of S, such that $\sigma(S,T) \geq \mu(T) > 0$ when $T < T_c$. Moreover, $\mu(T) \to 1$ as $T \to 0$.

Model 2: For each $\alpha < 1$ there is a $T_c(S) > 0$ and a function $\mu(S,T)$ such that $\sigma(S,T) \geq \mu(S,T) > 0$ when $T < T_c(S)$. $\mu(S,T) \to 1$ as $T \to 0$, but $T_c(S) \to 0$ as $S \to \infty$.

Model 3: For each S there is an $\alpha_c(S)$, with $0 < \alpha_c(S) < 1$, such that, for fixed $\alpha < \alpha_c(S)$, there is a function $\mu(S,T)$ and a T_c with the property that $\sigma(S,T) \geq \mu(S,T) > 0$ when $T < T_c$. Moreover $\alpha_c(S) \to 1$ as $S \to \infty$, and $\mu(S,0) \geq \frac{1}{3}$ with $\mu(S,0) \to 1$ as $S \to \infty$. Note that long-range order $[\sigma(S,T) > 0]$ implies that there are pure phases with spontaneous magnetization (or staggered polarization).

There are two principal parts to our proof. As in the Peierls argument[3] we want to show that the probability of a contour γ is small, i.e.,

$$D(\gamma) \equiv \langle P_\gamma \rangle$$

is small. Here P_γ is the projection onto the subspace in which all spins just inside (outside) γ have negative (positive) z component. Our first step is to relate $D(\gamma)$, which is a number of order unity, to an extensive quantity. The inequality is

$$D(\gamma) \leq \overline{\lim_{\Lambda \uparrow Z^2}} \langle P \rangle_\Lambda^{|\gamma|/4N},$$

where $|\gamma|$ is the length of γ and N is the number of sites in Λ. P is the projection onto the subspace of states in which every spin has either a positive or negative z component, and, in cases 1 and 2, the first two rows of spins must have positive z component, the next two rows have negative z component and so on, alternately. In case 3 the signs are reversed on one of the two sublattices.

The second step is to show that

$$D \equiv \overline{\lim_{\Lambda \uparrow Z^2}} \langle P \rangle_\Lambda^{1/N}$$

is small when T is small. We write

$$\langle P \rangle_\Lambda = \textstyle\sum_j \langle \varphi_j, P\varphi_j \rangle \exp(-e_j/kT)/Z_\Lambda,$$

$$Z_\Lambda = \textstyle\sum_j \exp(-e_j/kT),$$

where φ_j and e_j are the eigenvectors and eigenvalues of $H^{(\Lambda)}$. If e_0 is the ground-state energy, the terms in the numerator in which $e_j > e_0 + \epsilon N$, for $\epsilon > 0$, are easy to dispose of, because they have a small Boltzmann factor, i.e., they give a small contribution for energetic reasons. The terms with e_j close to e_0 present a difficulty. Classically they *vanish*, but in the quantum case one needs an estimate showing that states of low energy have small projections onto states which have a large H^z energy. This cannot be inferred by energetic considerations alone. We have proved a theorem which we call "exponential localization of eigenvectors." In the case at hand it says roughly that when $e_j < e_0 + \epsilon N$ then $\langle \varphi_j, P\varphi_j \rangle \leq a^d$, where $a < 1$ and d is the number of times H^{xy} must be applied to a state specified by P such that the resulting state has H^z energy less than $e_0 + \gamma N$, with γ small. Using this, it is possible to show that $D \to 0$ as $T \to 0$.

To summarize our results, we have established that quantum fluctuations are unimportant for the anisotropic ferromagnet and hence that some kind of spin-wave theory may be applicable. In the antiferromagnetic case, quantum fluctuations are unimportant if S is large enough (depending on α), but the situation for small S has not been decided rigorously.

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Temperature Dependence of the *K* X-Ray Emission Edge of Li†

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The *K* x-ray emission spectrum of Li has been measured with 0.1-eV resolution for temperatures between 85 and 490 K. A prominent shoulder is observed on the emission edge that is strongly broadened and shifted in energy as the temperature is raised. The peak in the emission spectrum lies about 0.6 eV below this shoulder. The steep high-energy edge of the spectrum is interpreted as a Fermi edge centered at 54.8 eV and having a width of 0.2 eV. The results are compared with similar structure observed in the absorption spectrum of Li.

The interpretation of the *K* x-ray edge of Li has long been a source of controversy. Both the soft x-ray emission (SXE)[1-6] and soft x-ray absorption (SXA)[7-9] edges have been measured by several workers. In emission data, there has been conflicting evidence as to whether the true emission spectra shows a steep high-energy edge with a peak at lower energies[1,4,6] or a gradual fall over about 0.8 eV from the peak of the emission spectrum.[2,3,5] It has been suggested that the steep edge is an experimental artifact which results from self-absorption.[10] This implies that the entire region above the peak in energy may be a very broad emission edge. On this assumption several theoretical attempts have been made to account for this very broad edge in terms of many-body effects[11-15] and lattice vibrations,[16-18] but the calculations have usually shown that the processes considered give much smaller edge broadening.

Considerable light was thrown on the Li edge problem recently by the measurements of Petersen and co-workers[7-9] who measured the SXA edge at temperatures from 4 K to above the melting point of Li (> 450 K) with good resolution (0.11 eV). At low temperatures they find a clear shoulder in the absorption edge.[7,9] They interpret the steeply rising region below the shoulder as the true Fermi edge. Their temperature studies indicate that the broadening (~ 0.2 eV at 80 K) of this edge is due predominantly to processes involving lattice vibrations.[8,9] A similar conclusion was reached by Baer, Citrin, and Wertheim[19] in their analysis of x-ray photoemission results. Following a suggestion by McAlister[10] which was based on an augmented-plane-wave (APW) band structure calculation, Petersen and Kunz attribute the peak above the shoulder to a peak in the one electron transition density located about 0.5 eV above the Fermi edge.

We have performed complementary experiments to those of Petersen and Kunz, measuring the soft x-ray emission spectra of Li with a resolution of 0.1 eV at a number of temperatures between 85 and 490 K. Our results are nearly a mirror image of theirs. A shoulder is present on the SXE edge at low temperatures that is broadened and shifted in energy by phonon processes as the temperature is raised. A peak is found about 0.7 eV below the Fermi edge. Our results show that the steep high-energy edge is not an artifact due to self-absorption, but represents the true Fermi edge. They also demonstrate that many of the differences in previous data can be attributed to differences in the temperature of the emitting cathode; the sharp edge observed at low temperatures[1,6] is washed out at higher temperatures. The results are important because they should serve to concentrate theoretical interest on the origin of the peak in the emission