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Magnetization of the anisotropic Heisenberg ferromagnet on a square lattice

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Abstract. A real-space renormalization group method which allows the direct calculation of the order parameter for magnetic systems is extended to quantum problems. The procedure is applied to the spin-$\frac{1}{2}$ Heisenberg ferromagnet on a square lattice in the presence of an Ising-like anisotropy. The results obtained are satisfactorily compared with experimental data on uncoupled ferromagnetic thin films in the monolayer range.

Phase transitions in quantum systems have been treated within the real-space renormalization group (RG) frameworks (see, for a review, [1]) over recent years. The Heisenberg ferromagnet and variations of it had been treated through RG by many workers [2–7], mainly regarding its phase diagram and thermal critical exponents. It is also desirable to obtain the thermodynamic functions for these quantum problems. In fact, RG methods are available [8, 9] for calculating the free energy, and through it the other thermodynamic functions, for arbitrary values of the external parameters. However, these procedures tend to be operationally heavy. In order to make the calculations easier, a simple RG formalism was introduced [10], which yields directly (without going through the calculation of the free energy) the order parameter for arbitrary temperatures T.

In the present work, an extension of this formalism to quantum systems is applied to the spin-$\frac{1}{2}$ anisotropic Heisenberg ferromagnet on a square lattice. This is an interesting problem not only from the theoretical point of view but also because of its possible relation [11] to uncoupled ferromagnetic films in the monolayer regime, such as epitaxial overlayers of Fe on Au(100) and polycrystalline layers of Permalloy (80% Ni–20% Fe) on Ta [12]. The main features of the magnetization of these uncoupled films are an initial decrease in the magnetization with increasing T slower than the decrease which the spin-wave theory predicts [13] and a sharp drop in the magnetization as the critical temperature is approached. The lack of low-energy magnetic excitations in the uncoupled films has been suggested [12] to be a universal property of ultrathin ferromagnetic films, independent of substrate, film material and crystalline structure.

Let us now consider the dimensionless Hamiltonian

$$H = \sum_{\langle i,j \rangle} K[(1 - \Delta)(\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y) + \sigma_i^z \sigma_j^z] \tag{1}$$

where $K = J/k_B T$ and the summation runs over all pairs of nearest-neighbour sites on a

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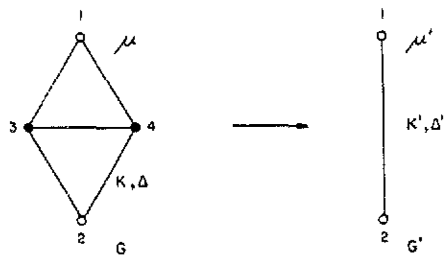

Figure 1. Clusters used to construct the RG transformation for the square lattice: ●, internal (root) sites; ○, terminal (root) sites.

square lattice. The σ-matrices are the standard Pauli matrices associated with spins $\frac{1}{2}$ and Δ is the anisotropy in spin space. The particular cases $\Delta = 1$, $\Delta = 0$ and $\Delta = -\infty$ correspond, respectively, to the Ising, isotropic Heisenberg and XY models.

Following along the lines of [10] in order to find the equation for the order parameter, an elementary dimensionless magneton μ is associated with each site of a d-dimensional lattice of linear size L; K and Δ are associated with each bond of this lattice. The order parameter is defined, in the $L \to \infty$ limit, as $M = N_L(K, \Delta)/L^D$. $N_L(K, \Delta)$ is the thermal canonical average number of sites whose spin z-projection is pointing in the easy-magnetization direction minus those whose spin z-projection is in the opposite direction. This system of L^D sites is renormalized into L'^D cells, each of linear size $B = L/L' > 1$. The variables K', Δ' and μ' associated with this new system can be expressed in terms of the old variables. The order parameter is now $M(K', \Delta') = N_{L'}(K', \Delta')/L'^D$. Any component of the total magnetic moment (extensive quantity) must remain the same in both original and renormalized systems:

$$N_{L'}(K', \Delta')\mu' = N_L(K, \Delta)\mu. \tag{2}$$

Equation (2) implies, following the same steps as in [10], that, for a point (K, Δ) belonging to the ordered phase,

$$M(K, \Delta) = \lim_{n\to\infty} (\mu^{(n)}/B^{nD}) \tag{3}$$

with n the number of iterations of the RG procedure. If the point belongs to the disordered phase, equation (2) implies that $M(K, \Delta) = 0$, as desired.

Equation (3) has to be used together with the RG recursion relations for K, Δ and μ. The equations for K and Δ used here were obtained in [14]. The formalism [14, 15] is cluster based, in which two-rooted graphs are used (see, for example, the transformation in figure 1, which is adopted here and is associated [10] with $B^D = 5$). This procedure is briefly outlined in the following. If a graph G is renormalized into a smaller graph G′, the correlation function between the two terminals of the graphs must be preserved. For the transformation of figure 1,

$$\exp(H'_{12}) = \mathop{\mathrm{Tr}}_{3,4} [\exp(H_{12324})] \tag{4}$$

with H_{1234} the Hamiltonian of equation (1) with $\langle i, j\rangle = \langle 1,3\rangle, \langle 3,2\rangle, \langle 1,4\rangle, \langle 4,2\rangle$ and $\langle 3,4\rangle$, associated with G, and

$$H'_{12} = K'[(1-\Delta')(\sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y) + \sigma_1^z\sigma_2^z] + K'_0 \tag{5}$$

associated with G′. K'_0 is a constant which allows equation (4) to be possible. To find

K', Δ' and K'_0 as functions of K and Δ, the first step is to find the exact form of the expansions of $\exp(H_{1234})$ and $\exp(H_{12})$. They are reproduced here, from [14]:

$$\exp(H'_{12}) = a' + b'_{12}(\sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y) + c'_{12}\sigma_1^z\sigma_2^z \tag{6a}$$

where the coefficients a', b'_{12} and c'_{12} depend on K', Δ' and K'_0, and

$$\begin{aligned}\exp(H_{1234}) = a + \sum_{i<j} [&b_{ij}(\sigma_i^x\sigma_j^x + \sigma_i^y\sigma_j^y) + c_{ij}\sigma_i^z\sigma_j^z \\ &+ d_{ij}(\sigma_i^x\sigma_j^x + \sigma_i^y\sigma_j^y)\sigma_k^z\sigma_l^z + e_{ij}(\sigma_i^x\sigma_j^x + \sigma_i^y\sigma_j^y)(\sigma_k^x\sigma_l^x + \sigma_k^y\sigma_l^y)] \\ &+ f\sigma_1^z\sigma_2^z\sigma_3^z\sigma_4^z\end{aligned} \tag{6b}$$

where the coefficients depend on K and Δ and $(k, l) \neq (i, j)$. Performing the trace of equation (4) on equation (6*b*) and comparing the result with equation (6*a*), relations between these coefficients are obtained. To find the explicit expressions of these coefficients in terms of K, Δ, K', Δ' and K'_0, what is done is to write the original and renormalized Hamiltonians matrices in a convenient basis and diagonalize them. For Heisenberg Hamiltonians the appropriate basis diagonalizes simultaneously all σ_i^z. By finding the diagonal forms of H'_{12} and H_{1234} it is possible to write $\exp(H'_{12})$ and $\exp(H_{1234})$ as matrices in which the elements are functions of K', Δ' and K'_0, and K and Δ, respectively. Finally it is necessary to express the expansions of $\exp(H'_{12})$ and $\exp(H_{1234})$ in the same basis as before. By comparing these matrices the coefficients a'_{12}, b'_{12} and c'_{12} are written as functions of K', Δ' and K'_0, as well as the coefficients a, $\{b_{ij}\}$, $\{c_{ij}\}$, $\{d_{ij}\}$, etc, are written as functions of K and Δ, as desired.

Through the procedure outlined above the RG relations for K and Δ were obtained in [14]. These relations yielded [14] a phase diagram which presents the correct Ising-type behaviour for $0 < \Delta \leqslant 1$. In the $\Delta = 1$ ($\Delta = 0$) limit the exact T_c ($T_c = 0$) was found. For other values of Δ, the critical temperatures are believed [14] to be a very good approximation.

Let us now introduce the procedure to find, in the quantum case, the RG recursion relation for μ. In order to break the symmetry, the z-component of the spin at one of the terminals of both graphs G and G′ is fixed. The other spins are completely free. Each cluster configuration will be weighed with the corresponding Boltzmann factor and will be associated with a value for the z-component of the cluster magnetic moment m^z. Each site contributes to m^z of a given configuration proportionally to its coordination number [10]. The thermal canonical average of the z-component of the cluster magnetic moment must be preserved through renormalization. For the specific case here,

$$\langle m'^z_{12}\rangle = \langle m^z_{1234}\rangle \tag{7}$$

i.e.

$$\begin{aligned}&\mathrm{Tr}_2[\exp(H'_{12})\,(\sigma_1^z + \sigma_2^z)\mu']/\mathrm{Tr}_2[\exp(H'_{12})] \\ &\quad = \mathrm{Tr}_{2,3,4}[\exp(H_{1234})\,(2\sigma_1^z + 2\sigma_2^z + 3\sigma_3^z + 3\sigma_4^z)\mu]/\mathrm{Tr}_{2,3,4}[\exp(H_{1234})].\end{aligned} \tag{8}$$

In this equation, the expansions of equations (6*a*) and (6*b*) are used. Equation (8)

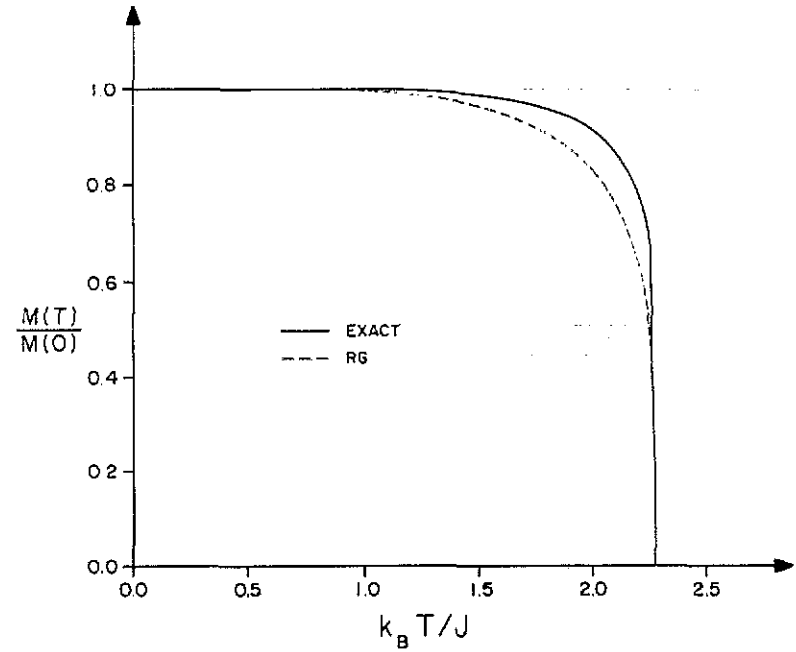

Figure 2. Normalized magnetization $M(T)/M(0)$ as a function of the normalized temperature $k_B T/J$ obtained for the Heisenberg ferromagnet with $\Delta = 1$ (– – –) compared with the Ising exact result (——).

determines the recursion relation for μ. The expressions that we have calculated for the cluster magnetic moments are

$$\langle m'^{z}_{12}\rangle = [(a' + c'_{12})/a']\mu' \tag{9a}$$

$$\langle m^{z}_{1234}\rangle = [(2a + 6c_{13} + 2c_{12})/a]\mu. \tag{9b}$$

These equations expressed as functions of K, Δ, K', Δ' and K'_0 are

$$\langle m'^{z}_{12}\rangle = [2\exp(K' + K'_0)\,\mu']/\{\exp(K' + K'_0) + \exp(-K' + K')\cosh[2K'(1-\Delta')]\} \tag{10a}$$

$$\begin{aligned}\langle m^{z}_{1234}\rangle = \{&10\exp(5K) + 4\exp[K(1-\Delta)]\,[A\cosh(KA) - \Delta\sinh(KA)]/A \\ &+ 2\exp(-3K + 2K\Delta) - \exp[-K(1+\Delta)]\,[B\cosh(KB) \\ &- (2-\Delta)\sinh(KB)]/2B - \exp(-3K)/2\}\mu/\{\exp(5K) \\ &+ \exp[K(1-\Delta)]\,2\cosh(KA) + \exp(K) + 2\exp(-3K + 2K\Delta) \\ &+ \exp[-K(1+\Delta)]\cosh(KB) \\ &+ \exp(K - 2K\Delta)/2 + \exp(-3K)/2\}\end{aligned} \tag{10b}$$

with $A = [\Delta^2 + 16(1-\Delta)^2]^{1/2}$ and $B = [(2-\Delta)^2 + 32(1-\Delta)^2]^{1/2}$.

The spontaneous magnetization that we obtain for $\Delta = 1$ is compared with the exact (see, e.g., [16]) magnetization for the Ising model in figure 2. For intermediate

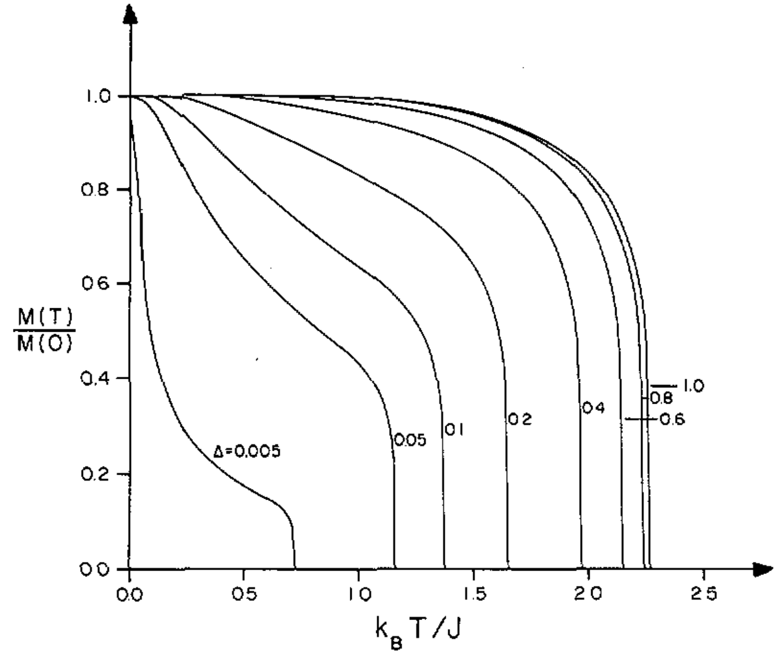

Figure 3. Normalized magnetization $M(T)/M(0)$ as a function of the normalized temperature $K_B T/J$ for $\Delta = 1, 0.8, 0.6, 0.4, 0.2, 0.1, 0.05$ and 0.005.

temperatures the error is of the order of 10%. The results obtained for the magnetization for $\Delta = 1, 0.8, 0.6, 0.4, 0.2, 0.1, 0.05$ and 0.005 are presented in figure 3. By comparing the present results and the RG results obtained in [11], it is found that in both cases the magnetization curves have the same shape but, as the critical temperatures in [11] are lower (owing to the approximation used), their curves are compressed.

In the neighbourhood of the critical point, the magnetization is given by $M \sim (1 - T/T_c)^\beta$. The exponent β is independent of the value of Δ ($\Delta \neq 0$), as expected on the basis of universality arguments: $\beta = 0.197$. This value must be compared with the Ising exact value, $\beta = 0.125$. Our β is not in good agreement with the exact result, probably because of the small cluster used. Other RG estimates for the 2D Ising exponent β using small clusters are, for example, $\beta = 0.180$ [10] and $\beta = 0.168$ [17]. In our case, better estimates will probably be obtained if the cluster size was increased, similarly to what was shown in [10] for the classical version of this method; as the size of the clusters increases, the calculated β approaches the exact result.

The asymptotic behaviour at low temperatures has been checked. It follows the exponential form $M \sim 1 - C\exp(-FJ\Delta/k_B T)$, for $\Delta \neq 0$, expected when there is a gap in the magnon spectrum. C and F are constants; $C = 0.3$ and $F = 4.9$ in this approximation. Only when $\Delta = 0$ does this gap vanish, since it is due to the anisotropy. This asymptotic behaviour is valid for $k_B T \ll \Delta J$. Even for very low values of Δ ($\Delta \neq 0$) this happens, but only in a small range of temperatures. In fact, if we want to see this in figure 3 for $\Delta = 0.005$, for instance, an amplification of scale would be necessary.

When Δ goes to zero, the magnetization must vanish at any finite T. One would naively think that the system will approach this limit simply by reducing T_c, without

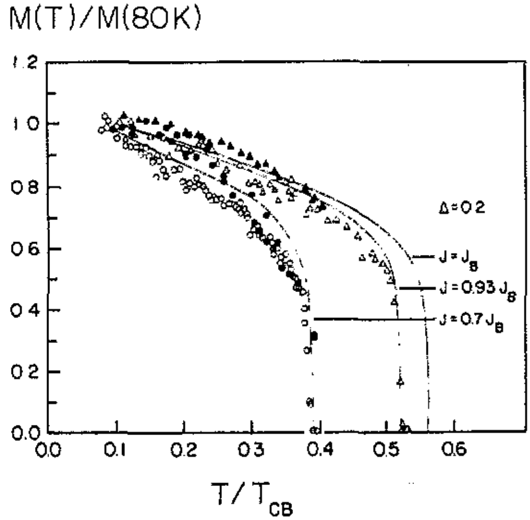

Figure 4. Spin polarization $P(T)$, normalized to $P(80\ K)$, for Fe on Au(100) and for Permalloy on Ta [12], as a function of the temperature normalized to the critical bulk temperature T_{CB}: ○, 1.8 monolayers of Fe; Δ, 2.5 monolayers of Fe; ●, 1.6 monolayers of Permalloy; ▲, 2.6 monolayers of Permalloy; ——, present results for $M(T)/M(80\ \mathrm{K})$ for $\Delta = 0.2$ and three different ratios of J/J_B.

changing the shape of the magnetization curve. As shown in figure 3, the situation for $\Delta = 0.05$ and $\Delta = 0.005$ clearly is not that one. A possible explanation is the following. For low values of Δ and low T, the easiest (low energetic cost) spin excitations are in the form of collective spin waves. At the criticality, however, the system has Ising character (as can be seen from the RG flux to the Ising attractor on the phase diagram) and there is a change in the nature of the excitations (now spin flips). This gives rise to a change in the magnetization behaviour between these two regimes. For higher values of Δ, at low T, the predominant excitations would be in the form of spin flips ($\Delta = 1$ is an extreme example), implying that there is not such a change of regime when T goes to T_c. We recall that a similar magnetization behaviour has already been found [18] for an anisotropic XY ferromagnet on a two-dimensional lattice. In [18], both classical and quantum versions of this model were treated; the only qualitative difference between them is the derivative of the magnetization in the zero-temperature limit, which was zero for the quantum case, as in the present results (for $\Delta \neq 0$).

In figure 4 the temperature dependences of the low-energy cascade spin polarization $P(T)$ normalized to the polarization measured at $T = 80$ K (assumed to be proportional to $M(T)/M(80\ K)$) of epitaxial overlayers of Fe on Au(100) and polycrystalline layers of Permalloy on Ta [13] are shown. These experimental data appear together with the present results for $\Delta = 0.2$, for three different ratios J/J_B (J is the exchange coupling of the 2D system and J_B is the isotropic bulk coupling, calculated in the third reference of [3]: $K_{CB} = J_B/k_B T_{CB} = 2.91$). The data agree remarkably well with the present theoretical results. In fact, the low value of Δ obtained confirms the belief [12] that these films are associated with weak anisotropies. In this way, the Heisenberg model in 2D reproduces the experimentally observed slower decrease in or even constancy (for higher values of Δ) of $M(T)$ at low T for uncoupled ferromagnetic films in the monolayer range.

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