SOLUBLE EXTENSION OF THE ISING MODEL

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In this note we wish to relate a somewhat trivial, but surprising, soluble extension of the multidimensional Ising model. Our extension was motivated by recent experiments on a real material, dysprosium aluminum garnet (DyAlG), which closely resembles an ideal three-dimensional Ising model,[1] except for what appeared to be one unfortunate detail: The electronic (Ising) spins are connected not just to their electronic neighbors, but also to their own dysprosium nuclei by a fairly large hyperfine interaction. The interacting nuclear isotopes are randomly distributed with a natural abundance of 18.9% for Dy^{161} (hyperfine coupling constant $A = 0.073°K$) and 25% for Dy^{163} ($A = 0.104°K$).[2] This physical system thus corresponds to a model Ising antiferromagnet disturbed by a magnetic field (the hyperfine-coupled nuclear spins) random in magnitude and position. The magnitude of the disturbance is not negligible, considering the low critical temperature of DyAlG ($T_N = 2.5°K$), and is indeed comparable in magnitude with any one of the Ising bonds!

Given this substantial random perturbation of the Ising spins, it is reasonable to expect a drastic effect on thermodynamic properties, especially critical-point phenomena. For example, an estimate on the basis of molecular field theory shows each spin in a different specific environment, and hence a broadening of the transition region. The smallest effect on the thermodynamic properties which one might reasonably expect is a broadening of the lambda point, or perhaps a change in the order of the phase transition.

The experiments[1] show no such thing! On the contrary, the usual type of logarithmic peak is found to within about 3×10^{-3} °K of the Néel point. We studied this problem theoretically, and discovered that this was no accident. We shall show that the thermal properties of the perturbed system can be related exactly to the properties of an ideal Ising model without requiring any knowledge of the latter. This is fortunate because, apart from various numerical estimates,[3] no solution of the three-dimensional Ising model in closed form is known at the present time. However, even without such a solution, we easily prove that the singularity at T_N and other critical-point phenomena are essentially the same in the perturbed system as in the ideal one, and that the two will differ only by smoothly varying nonsingular functions of temperature.

If we denote the nuclear spins by I_i and electron (Ising) spins by σ_i, spin-spin interactions by J_{ij}, and the hyperfine bonds by A_i, the total Hamiltonian $\mathcal{H}$ is

$$\mathcal{H}=\mathcal{H}_0+\tfrac{1}{2}\sum_i A_i\sigma_i^z I_i^z, \tag{1}$$

where $\mathcal{H}_0$ is the ideal Ising Hamiltonian,

$$\mathcal{H}_0=\sum_{(ij)} J_{ij}\sigma_i^z\sigma_j^z-\mu H\sum_i \sigma_i^z, \tag{2}$$

and we neglect the extremely small direct interactions between the nuclear spins themselves and with the external field. The Ising spins have only two values, $\sigma_i^z=\pm1$, but the nuclear spins may have various magnitudes I_i (including $I=0$), depending on which isotopic species is at the ith site. For the case of Dy, $I=\frac{5}{2}$ for the two isotopes Dy^{161} and Dy^{163} and $I=0$ for all other isotopes.

We now note that the partition function of the combined system, $Z=\mathrm{Tr}\{\exp(-\beta\mathcal{H})\}$, may be evaluated in two steps, decomposing the grand trace into a partial trace over the nuclear spins only, Tr_I, followed by a trace over electron spins Tr_σ.[4] Using the fact that only even powers in $(I_i^z)^n$ contribute to Tr_I and that $(\sigma_i^z)^{2n}\equiv1$, we find

$$Z=\mathrm{Tr}_\sigma\{\exp(-\beta\mathcal{H}_0)\}\,\mathrm{Tr}_I\{\exp(-\beta\textstyle\sum_i\frac{1}{2}A_iI_i^z)\}$$
$$=Z_0Z_I, \tag{3}$$

where Z_0 is the partition function of the unperturbed Ising system and Z_I a nuclear partition function independent of the electron spins identically equal to the partition function of the same nuclei in fixed external fields A_i. Z_I is a smoothly varying, continuous function of temperature and any singularities in the electron-spin system will thus be unaffected by the presence of the nuclear spins, no matter how large their coupling to the electron spins may be! In particular, the nuclei will leave T_N unchanged and they will simply add a smoothly varying term to the Ising specific heat $C_0(T)$:

$$C(T)=C_0(T)+\sum_i \tfrac{1}{2}A_iI_i\frac{d}{dT}B_i(\beta A_i/2), \tag{4}$$

where $B_i(x)$ is the Brillouin function appropriate to a spin I_i. This contribution is smooth and analytic and the nature of the singularity is therefore unaffected in all respects! It is doubtful whether the present authors would have sought, and found, this exact result had the experiments not indicated it first. Our results do not preclude the possibility that part of the broadening of the transition observed in other non-Ising-like materials[5] may in fact be due to random nuclear fields. In this connection it would be interesting to show whether or not the small width of the specific-heat peak observed in DyAlG ($\sim3\times10^{-3}$ °K) is in fact due to the finite non-Ising-like terms ($A\times\sigma\times I\times$etc.) in the hyperfine interaction.

It is now simple to extend the above method of splitting the traces to predict the behavior of the nuclear-spin system. For the average nuclear magnetization we find

$$\langle I_i^z\rangle=Z^{-1}\,\mathrm{Tr}_\sigma\{\exp(-\beta\mathcal{H}_0)$$
$$\times\mathrm{Tr}_I[I_i^z\exp(-\beta\textstyle\sum_n\frac{1}{2}A_n\sigma_n^zI_n^z]\}$$
$$=I_iM_0(T)B_i(\beta A_i/2), \tag{5}$$

where $M_0(T)$ is the electron sublattice magnetization, which vanishes above T_N. Below T_N we may also expect a correlation between different nuclei via the electronic spins, and we find for the long-range order

$$\langle I_n^zI_m^z\rangle=a_{mn}I_mI_nB_m(\beta A_m/2)B_n(\beta A_n/2), \tag{6}$$

where a_{mn} is the electron-spin order parameter in the absence of the nuclear spins,

$$a_{mn} = Z_0^{-1} \operatorname{Tr}_\sigma \{\sigma_m^z \sigma_n^z \exp(-\beta \mathcal{H}_0)\}. \qquad (7)$$

With the hyperfine interactions appropriate to Dy in DyAlG, this nuclear antiferromagnetic order should become appreciable below about 0.1°K.

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[1]B. E. Keen, D. Landau, and W. P. Wolf, to be published. For a summary of earlier work see W. P. Wolf, in Proceedings of the International Conference on Magnetism, Nottingham, England, 1964 (The Institute of Physics and the Physical Society, University of Reading, Berkshire, England, 1965), p. 555.

[2]Values of A calculated from the observed electronic g value and the results of A. H. Cooke and J. G. Park, Proc. Phys. Soc. (London) 69, 282 (1956), assuming the ratio A/g to be the same for Dy^{3+} in the acetate and the garnet.

[3]See, for example, M. E. Fisher and M. Sykes, Physica 28, 939 (1962).

[4]A similar factorization has previously been used by M. E. Fisher, Phys. Rev. 113, 969 (1959), in connection with decoration extensions of Ising models.

[5]See, for example, J. Skalyo, Jr., and S. A. Friedberg, Phys. Rev. Letters 13, 133 (1964); P. Heller and G. B. Benedek, Phys. Rev. Letters 8, 428 (1962); T. Yamamoto, in Proceedings of the International Conference on Phenomena in the Neighborhood of Critical Points, Washington, D. C. (to be published).