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Earlier calculations /1/, referred to as I of the thermodynamic properties of a Schrödinger spin-exchange ferromagnet are extended by considering the quadrupole moment, Q, for spin 1 systems.

The Schrödinger spin-exchange Hamiltonian relevant to an isotropic system in the constant-coupling approximation (CCA) is

$$H = -JP_{12} - \mu H(S_{1z} + S_{2z}) \ ,$$

where μ is the magnetic moment per spin, H is the internal and/or external magnetic field, and

$$P_{12} = (S_1 S_2)^2 + S_1 S_2 - 1 \quad \text{for } S = 1 .$$

The internal field can be found by calculating the average spontaneous magnetization, m, and equating it to the magnetization, m', found by using a one-spin Hamiltonian (molecular field approximation or MFA) with an internal field H'. The assumption that

$$\frac{H'}{n} = \frac{H}{n-1} \ ,$$

where n is the coordination number of the lattice, has been shown to be equivalent to the CCA /2/.

When the quadrupole moment is included, evaluating Q' and Q for the one- and two-particle systems and setting them equal will also evaluate the internal field but it will not be the same field found from requiring m and m' to be equal. It will be assumed that the proper field to use is the one that minimizes the free energy which, it can easily be shown, means the larger field in this case. Since the question of which field is larger depends on the temperature, this determines the phase diagram of the system.

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From I, the two-spin partition function is known to be

$$Z = 2e^{p}(1 + \cosh\lambda + \cosh 2\lambda) + e^{-p}(1 + 2\cosh\lambda),$$

where $p = \beta J$, $\lambda = \beta\mu H$, and $\beta = 1/kT$. Now,

$$m = \frac{1}{2}\frac{\partial \ln Z}{\partial \lambda} = \bar{m}$$

and

$$Q = \overline{m^2} - \frac{1}{3}S(S+1)$$

with corresponding definitions for m' and Q' in the one-spin system where

$$Z' = 1 + 2\cos h\lambda' .$$

The condition $m' = m$ gives a linear equation for e^{-2p} and $Q = Q'$, a quadratic in the same variable. Solving these equations then gives three values for the internal field as a function of temperature the knowledge of which allows all the thermodynamic properties to be evaluated. Aside from the quadrupole moment, these have been discussed in I.

The present work shows that the dipolar ferromagnetic state is preferred for all temperatures because the quadratic has no real solutions. The phase diagram is therefore quite simple: there is a paramagnetic (P) phase at high temperatures ($T > T_c$), a ferromagnetic (F) phase below ($T < T_c$), and no quadrupolar (Q) phase for any T.

To find other relevant theoretical predictions, we have to look to calculations using a biquadratic Heisenberg exchange Hamiltonian often written as

$$H = -2J\sum_{\langle ij\rangle}\left[S_i S_j + \alpha(S_i S_j)^2\right]$$

which, for $\alpha = 1$, is equivalent to the Schrödinger exchange except for a constant term and the factor two. The results of this comparison are mostly in agreement: using the MFA, Chen and Levy /3/ find a phase diagram which does indeed include a quadrupolar phase, although no F $\leftrightarrow$ Q transition, and the Q phase appears to occur only for $\alpha > 2$ (our α, not theirs). A Green's function approach /4/ shows that there is no Q phase since the quadrupole moment goes to zero at a temperature below T_c when the dipole moment vanishes for all α and, in particular, for $\alpha = 1$.

Another MFA calculation /5/ reaches the conclusion that dipolar ordering is always preferred and the Q phase does not exist, and another CCA calculation /6/ applied to an anisotropic Ising model also shows a phase diagram which suggests that there will be no Q phase for $\alpha = 1$.

Thus, although the evidence is rather meager, there is agreement from several theoretical sources that the system does not order as quadrupoles.

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