

On a Ferromagnetic with the Schrodinger Spin-Exchange Operator

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The properties of a ferromagnetic with a Hamiltonian using the Schrodinger spin-exchange operator are calculated. Most results are very reasonable but a disturbing difference exists between the Curie temperatures found by two different approximations.'

Calculam-se as propriedades de um meio ferromagnético utilizando-se uma hamiltoniana que inclui o operador de Schrodinger de troca de spin. A maioria dos resultados são razoáveis mas ocorre uma diferença inesperada na temperatura de Curie calculada em duas diferentes aproximações.

We present here a calculation of the properties of a ferromagnet with the two-particle Hamiltonian

$$H_{12} = -JP_{12} - g\beta HM, \quad (1)$$

where J is the two-particle exchange integral, P_{12} the spin-exchange operator', g the Landé factor, β the Bohr magneton, H the magnetic field, and M the z-component of the total spin of the two particles. Such a Hamiltonian has been suggested² as a possible alternative to the Heisenberg Hamiltonian usually used in theories of ferromagnetism and some of the resulting properties have been calculated for spin = 1^{2,3}. Calculations of the transition temperature and some other properties at higher temperatures have also been carried out for higher spins⁴.

In the present note, we choose the spin to be $S_0 = 2$ and the method of calculation to be the well-known constant-coupling approximation⁵.

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We need to evaluate the partition function, summing over the eigenvalues of H_{12} . Since the eigenvalues of P_{12} are ± 1 , depending on the total spin, $S \leq 2S_0$, and those of M are between $-S$ and $+S$, the result is immediate:

$$Z = e^p [C_4(\lambda) + C_2(\lambda) + 1] + e^{-p} [C_3(\lambda) + C_1(\lambda)] \quad (2)$$

where

$$C_n(\lambda) = 1 + 2 \sum_{k=1}^n \cosh(k\lambda)$$

$$p = J/kT, \quad \lambda = g\beta H/kT, \quad H = H_0 + H_1,$$

with H_0 the applied field and H_1 the internal or Weiss field.

The internal field is evaluated by means of a consistency condition³: The partial trace over one spin of the two-particle density matrix must reduce to the one-particle density matrix with the internal fields in the two density matrices being in the ratio $(n-1):n$, where n is the coordination number of the lattice. The internal field is then calculated numerically from an implicit equation, giving the field as a function of the temperature (and the applied field).

At this point, the thermal properties of the system can be found and we proceed to calculate the Curie temperature, the magnetization, the susceptibility, and the exchange energy and specific heat. The results are summarized below.

The Curie temperature is taken to be that at which the magnetization goes to zero when there is no applied field. We find

$$p_c = J/kT_c = (1/2) \ln [(n+3)/(n-7)], \quad (3)$$

a result which is considerably different from that found by the high-temperature series expansion method⁴, as shown in Table 1.

n	kT_c/J	
	present calculation	series expansion ⁴
6	complex	?
8	.834	1.82
12	1.62	2.34

Table 1 - Reduced Curie temperatures for several lattices.

The average magnetization per atom, m , cannot be stated in explicit form, but we can obtain approximate values in the two limited regions:

$$\text{i) } T - 0: \quad m \approx 2 - [(1 + e^{-2p})/2]^n, \quad (4)$$

$$\text{ii) } T \rightarrow T_c: \quad m \approx [t(1-t)]^{1/2}. \quad (5)$$

Note the absence of complete saturation; m has the value $2 - (1/2)^n$ at absolute zero, a result typical of the constant-coupling approximation. Saturation is approached but never quite achieved. The temperature behavior in both regions is like that of the molecular field theory and many other cluster approximations.

For temperatures above T_c , it is not difficult to find the susceptibility per atom, and the exchange energy and heat capacity per atom is:

$$\chi = \frac{C}{T} \left[\frac{3 + 7 \exp(2p)}{(n + 3) - (n - 7) \exp(2p)} \right] \quad (6)$$

with

$$C = g^2 \beta^2 S_0(S_0 + 1)/3k, \quad (7)$$

$$E = -\frac{nJ}{2} \left[\frac{3/2 - \exp(-2p)}{3/2 + \exp(-2p)} \right],$$

$$c/K = \frac{3np^2 \exp(-2p)}{[3/2 + \exp(-2p)]^2} \quad (8)$$

Below T_c , these quantities, like the magnetization, can only be obtained numerically.

The inverse susceptibility will be almost a straightline with some positive curvature near T_c . For $T \gg T_c$, the Curie-Weiss law holds,

$$\chi = C/(T - \theta),$$

with the asymptotic Curie temperature given by

$$k\theta/J = (14 - n)/5 \quad (9)$$

and the ratio

$$\theta/T_c = [(14 - n)/10] \ln [(n + 3)/(n - 7)], \quad (10)$$

or 1.44 for $n = 8$ and 1.26 for $n = 12$.

The heat capacity shows a tail above T_c that eventually falls off as T^{-2} .

The behavior of these functions is quite typical of several theoretical methods that improve on the molecular field theory.

Because of this similarity of the present results to those of other theoretical approaches, and the qualitative agreement with experimental data, it does not seem possible to state definitively the utility or not of the Hamiltonian proposed in **Eq. (1)**.

On the other hand, the large discrepancy in the values of kT_c/J found by the present constant-coupling calculation and those found by the high-temperature series expansion method⁴ suggests the possibility of some difficulty. Both theoretical methods are known to be usually trustworthy and to give quite similar results⁶. One has an uneasy feeling on finding that two different, usually reliable methods give such dissimilar results. The fault could lie in the proposed Hamiltonian or in the applicability of either approximation to that model.

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References and Notes

1. E. Schrodinger, Proc. Roy. Irish Acad. 47, 39 (1941).
2. G. A. T. Allan and D. D. Betts, Proc. Phys. Soc. (London) 91, 341 (1967).
3. H. A. Brown, Phys. Rev. B 4, 115 (1971).
4. H. H. Chen and R. I. Joseph, Solid State Comm. 8, 459 (1970).
5. P. W. Kasteleijn and J. van Kranendonk, Physica 22, 317 (1956) see also Ref. 3.
6. In particular, for $S_0 = 1$, we find from Refs. 2 and 3 that $kT_c/J = 6.46$ and 6.14 for $n = 12$. about a 5% difference.