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Note on the Second or Gaussian Approximation in the Heisenberg Theory of Ferromagnetism When $S > \frac{1}{2}$

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IN the Heisenberg theory, it is customary, except at very low temperatures, to write the expression for the intensity of magnetization in the form

$$M = Ng\beta B_1(g\beta p H + apJ + bp^2J^2 + \dots), \quad (1)$$

where J is the exchange integral, β is the Bohr magneton, H is the applied field, and

$$p = 1/kT, \quad B_n(\theta) = \sum_{m=-S}^{+S} m^n e^{-m\theta} / \sum e^{-m\theta}. \quad (2)$$

Eq. (1) shows that $(aJ + bpJ^2 + \dots)/g\beta$ plays the role of an internal or "molecular" field. The coefficients a, b, \dots are functions of M . It is quite easy to prove, as has often been done, that

$$a = 2zM/Ng\beta, \quad (3)$$

where z is the number of neighbors. The evaluation of b involves the second or so-called Gaussian approximation, since it can be shown that (1) would be exact, without the unwritten higher order terms, were the energy values for a given spin distributed in accordance with a Gaussian error law. If $S = \frac{1}{2}$, then a calculation made either by means of group theory¹ or the vector model² shows that

$$b = -(2zM/Ng\beta) + (4zM^3/N^3g^3\beta^3). \quad (4)$$

The proper formula for b has not previously been given when $S > \frac{1}{2}$, as neither method can be used for this purpose,³ at least in a simple way, except when $S = \frac{1}{2}$.

A quite different approach has, however, recently been developed by Opechowski.⁴ He develops the partition function as a power series in J . The constant b in (1) is uniquely fixed by the requirement that the expansion of (1) agree with

this series development to J^2 inclusive. Opechowski shows that in this way formula (4) can be derived quite easily when $S = \frac{1}{2}$. His work reveals perhaps more clearly than does the ordinary calculation by means of an assumed Gaussian spread,⁵ that the practical convergence of the form (1) is very poor at ordinary temperatures. Indeed, better agreement with experiment is usually obtained if one stops with apJ than if one includes bp^2J^2 , or, as he shows, even dp^4J^4 .

It is the purpose of the present note to show that the calculation of the partition function which I gave in a previous paper on ferromagnetic anisotropy⁶ permits extension of the results to arbitrary S . Also it is well to mention that the general mathematical procedure which I used is in many respects similar to that employed by Opechowski, although obtained independently. The essence of both schemes was the development of the partition function in a system of representation in which each atom is separately space quantized in a field H . Because of the invariance of the diagonal sum, use of such a system is allowable even with interatomic perturbations. Saturation effects are not overlooked, and so H can be arbitrarily large. In one notable respect, Opechowski's calculations are more general than ours, as he carries the development far enough to include third and fourth powers of the exchange integral, corresponding to unwritten terms $cp^3J^3 + dp^4J^4$ in (1). On the other hand, my computation, though carried less far, was made for arbitrary S , and allowed the interaction between atoms to be of the dipole-dipole rather than exchange type if desired. The introduction of dipole-dipole coupling is obviously not needed in connection with the present note, but was wanted for other purposes, and somewhat complicates the mathematics, as it makes the perturbing potential cease to commute with the main or Zeeman energy.

¹ W. Heisenberg, *Zeits. f. Physik* **49**, 619 (1928).

² J. H. Van Vleck, *The Theory of Electric and Magnetic Susceptibilities*, Chap. XII.

³ See especially footnote 16, p. 329 of reference 2.

⁴ W. Opechowski, *Physica* **4**, 181 (1937).

⁵ Cf., however, D. Inglis, *Phys. Rev.* **42**, 442 (1932).

⁶ J. H. Van Vleck, *Phys. Rev.* **52**, 1190 (1937).

For arbitrary S , to terms in J^2 , the formula for the magnetic moment is

$$\begin{aligned} M/Ng\beta = & B_1 + 2zpJB_1(B_2 - B_1^2) \\ & + zp^2J^2(B_2 - B_1^2)(-8zB_1^3 \\ & \quad + 4zB_1B_2 + 4B_1^3 - 4B_1B_2 - B_1) \\ & + zp^2J^2(B_3 - B_1B_2)(2zB_1^2 - 2B_1^2 + B_2 - S^2 - S). \end{aligned} \quad (5)$$

Eq. (5) is derived from my previous expression for the partition function in almost exactly the same way as is Eq. (3) of my article on adiabatic demagnetization appearing in the present issue,⁷ to which the reader is referred for further detail. The only differences are that in (5) all dipole-dipole terms are omitted, and S is not specialized to the value $S = \frac{1}{2}$. In (5) the argument of the B functions is merely⁸ $g\beta p H$. On the other hand, in (1) it is $g\beta p H + apJ + bp^2J^2 \dots$, or to our degree of approximation

$$g\beta p H + 2zpJB_1 + 4z^2p^2J^2B_1(B_2 - B_1^2) + bJ^2,$$

as is seen from (3) and (5). By expanding (1), in essentially the same way as explained more fully on page 192 of Opechowski's paper,⁴ it is found that (1) and (5) are the same to J^2 provided

$$\begin{aligned} b = & z(4B_1^3 - 4B_1B_2 - B_1) \\ & + z(-2B_1^2 + B_2 - S^2 - S) \\ & \times (B_3 - B_2B_1)(B_2 - B_1^2)^{-1}. \end{aligned} \quad (6)$$

In Eq. (6), B_1 may be replaced by $M/Ng\beta$, as in the second-order coefficient b it is unnecessary to distinguish between arguments exclusive and inclusive of the inner field.

In the special case $S = \frac{1}{2}$, one has $B_3 = \frac{1}{4}B_1$,

⁷ J. H. Van Vleck, J. Chem. Phys. **6**, 81 (1938).

⁸ In the application to anisotropy in reference 6, an inner field was included in the argument of the B functions, but is to be omitted in deriving Eq. (5) from our previous calculations, as (5) is obtained by treating the exchange energy as part of the perturbing potential.

$B_2 = \frac{1}{4}$ and (6) reduces to the simple expression (4).

If $S = 1$, the following formulas apply

$$\begin{aligned} B_3 = B_1, \quad B_1 = & 2 \sinh \theta / (1 + 2 \cosh \theta), \\ B_2 = & 2 \cosh \theta / (1 + 2 \cosh \theta). \end{aligned} \quad (7)$$

By elimination of θ between the last two relations of (7), a quadratic equation is obtained giving B_2 in terms of $B_1 = M/Ng\beta$. It is thus possible to reduce (6) to an explicit function of M alone, but the resulting formula for b involves M through radicals and is too cumbersome to be of much value.

When $S > 1$, the interrelations between B_1 , B_2 , B_3 yielded by (2) are more complicated than (7). It is still possible, in principle, to express B_2 , B_3 in terms of B or M , but only by solving algebraic equations of high degree, *viz.* $2S$. The practical use of (6) thus appears to be limited to $S = \frac{1}{2}$ and possibly $S = 1$, unless the field is weak, as is the case above the Curie point. The limiting general form of (6) for weak fields is tractable, and has been given in a previous paper, as well as discussed in relation to the critical conditions for ferromagnetism.⁹ The rather unpleasant result (6) of a calculation of b for $S > \frac{1}{2}$ in arbitrary fields is of interest mainly in connection with the light which it throws on the failure of group theory or the simple vector model to furnish a method of computing b when $S > \frac{1}{2}$. Either of these procedures appear capable of yielding only an answer such as (4) which is a polynomial in M (or at least this is what analogy to the way they work for $S = \frac{1}{2}$ would suggest). Hence they must fail when $S > \frac{1}{2}$, since then the true formula for b is far from a polynomial.

⁹ J. H. Van Vleck, J. Chem. Phys. **5**, 320 (1937), especially footnote 20.