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SIGNIFICANCE of DIMENSIONALITY in the SPIN WAVE THEORY of FERROMAGNETISM

BY
HENRY UNRUH, JR.

U. S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

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Contents

The Significance of Dimensionality in the Spin Wave Theory of Ferromagnetism

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The significance of dimensionality in the magnetic properties of a single domain ferromagnetic system is determined utilizing a new approach to the spin wave theory and a few plausible assumptions. If conditions are such as to produce spontaneous magnetization in a finite temperature range for a specific dimensionality then under the same conditions there exists a finite temperature range for every dimensionality in which spontaneous magnetization occurs.

Key Words: Spin Waves, Linear chain, ferromagnetism.

1. Introduction

It has been claimed on the basis of the spin wave theory that spontaneous magnetization for one and two dimensional systems cannot occur in contrast to the three dimensional system[1]. In this regard, the ferromagnetic thin film has been the subject of both theoretical[2] and experimental[3, 4] investigation. The experimental results so far appear inconclusive. In this paper the dependence of the spontaneous magnetization on dimensionality is re-examined, paying particular attention to the role played by anisotropies such as that due to an externally applied field. The results are applicable in all dimensionalities if the low temperature limit is taken, and further, are applicable for unrestricted temperature in the one dimensional case if one makes a few plausible assumptions.

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2. Calculations

In what follows the Hamiltonian operator[5] is assumed for a system of N spins to be given by

$$\mathcal{H} = \mathcal{H}_1 - g\beta \underset{\sim}{H} \cdot \sum_{j=1}^{N} \underset{\sim}{S}_j \qquad (1)$$

with

$$\mathcal{H}_1 = -J \sum_j \sum_z \underset{\sim}{S}_j \cdot \underset{\sim}{S}_z \qquad (2)$$

where J is the exchange integral (effective only between nearest neighbors), $\underset{\sim}{H}$ is the field intensity and includes contributions from crystalline anisotropies, β is the Bohr magneton, g is the spectroscopic splitting factor and $\underset{\sim}{S}_j$ is the operator for the spin in the j position. The sum over z shall include only those spins nearest neighbor to j. The Heitler-London model of well localized spins is assumed. Only the case of spin ½ is considered.

For the operator (1) there exist eigenstates (in any dimensionality) with q spins directed downward, which have the form

$$\psi(N, q) = \sum_{m_1,\, m_2 \cdots m_q = 1} a(m_1,\, m_2 \cdots m_q)\, \alpha_1 \cdots \beta_{m_1} \cdots \beta_{m_q} \cdots \alpha_N \qquad (3)$$

where the sum is so restricted that two or more inversions cannot be located in the same position. The α's and β's represent the up and down states respectively while the subscript determines the position of the spin in the lattice. The eigenvalues of (1) belonging to (3) may conveniently be written [6, 7], aside from the unimportant constant $-\frac{Nz\,J}{4}$,

$$E(k_1,\, k_2 \cdots k_q) = 2J \sum_{\nu=1}^{q} (1 - \cos k_\nu) - \tfrac{1}{2} g\beta H(N - 2q) \qquad (4)$$

in which it is assumed that $\underset{\sim}{H}$ determines the preferred direction for the spin. The k_ν are restricted to certain values which are given exactly for any N and for $0 \leq q \leq \frac{1}{2}N$ in the one dimensional case, and approximately for $q << N$ in any dimension by Bethe.[6, 7]

From (4) one may obtain the magnetic moment according to

$$M(N, T, H) = \kappa T \frac{\partial \ln Z}{\partial H} \tag{5}$$

where κ is Boltzmann's constant, T is the absolute temperature and Z is the partition function.

The evaluation of (5) has been accomplished by approximate methods[7], usually with H = 0, and gave the results

$$M(N, T, 0) = \tfrac{1}{2} g \beta N(1 - \text{const } T^{3/2}) \tag{6}$$

for low T in the three dimensional case, and $M(N, T, 0) \rightarrow -\infty$ for any T in the one and two dimensional cases. These results are the basis for the statement that only the three dimensional system can be spontaneously ferromagnetic.

However, it appears that an improved value for M(N, T, H) which yields a different relationship between dimensionality and the magnetization can be obtained by separating out a part of Z which can be done exactly as is shown in the following steps.

Consider the operator $S^{\pm}$ defined by

$$S^{\pm} = \sum_{j=1}^{N} (S_j^x \pm S_j^y)$$

where S_j^x and S_j^y are the x and y components of $\underset{\sim}{S}_j$. Then

$$S^{-}\psi(N,q) = \sum_{f=1}^{N} \sum_{m_1,\, m_2 \cdots m_q = 1}^{N} a(m_1,\, m_2,\, \ldots\, m_q)$$

$$\times\ \alpha_1\, \alpha_2 \cdots \beta_f \cdots \beta_{m_1} \cdots \beta_{m_q} \cdots \alpha_N$$

that is--the operation by S^{-} increases the total number of inversions by one, and $a(m_1, m_2 \cdots m_q)$ is independent of the location of the new inversion, β_f, so introduced. It is understood that the sums are so restricted that two or more inversions cannot be located at the same point. Each repeated application of S^{-} introduces one more such inversion. It is now convenient to rewrite the eigenfunction, $\psi(N,q)$, in the form $\psi_h(N,r)$ in which h represents the number of inversions whose locations are independent of the $a(m_1 \cdots m_q)$, i.e. the indices which determine the location of the spins in the lattice do not appear in the $a(m_1 \cdots m_q)$, and there are r remaining ones so that $q = h + r$. What has just been established then is that

$$S^{-}\psi_h(N,r) = \psi_{h+1}(N,r).$$

In fact, if we suppose that we start with a state having $h = 0$ so that all of the indices locating the inversions appear explicitly in $a(m_1 \cdots m_r)$ we see that

$$\psi_h(N,r) = (S^{-})^h \psi_o(N,r).$$

At this point it would be convenient if one had established the correctness of the following two statements:

1. Those inversions, and only those, introduced by the S^{-} operator, i.e., all those inversions whose locations have no effect on the $a(m_1 \cdots)$ coefficients, each have an associated k value of zero.

2. That $S^{-}\psi_{N-2r}(N, r) = 0$.

The author believes that he has accomplished these proofs in general for the one dimensional case and is publishing them separately in National Bureau of Standards Technical Note No. 328,[8] since they are rather lengthy.

For the time being we prove and illustrate the use of the two statements for the case of one inversion in a linear chain and indicate some simple interpretations that may be made concerning the physical system.

For a linear chain with one inversion the a(m) coefficients are well known[5] so that the eigenstate may be expressed by

$$\psi = \sum_{j=1}^{N} e^{ikj} \alpha_1 \alpha_2 \cdots \beta_j \cdots \alpha_N$$

where k is restricted according to

$$k = \frac{2\pi \ell}{N}, \quad \ell = 0, 1, 2 \cdots N-1.$$

In the notation previously introduced we would write the eigenstate as $\psi_1(N, 0)$ if $k = 0$ and $\psi_o(N, 1)$ if $k \neq 0$. Of course, for $k = 0$ the location of the inversion has no effect on the coefficient, which is an illustration of statement one above.

Making use of the fact that

$$S^{+} \psi_o(N, 1) = \left(\sum_{j=1}^{N} e^{ikj} \right) \alpha_1 \alpha_2 \cdots \alpha_j \cdots \alpha_N = 0$$

and that

$$S^2 = S^{-}S^{+} + S^z + (S^z)^2$$

we see that

$$S^2\psi_o(N,1) = \gamma\psi_o(N,1), \text{ where } \gamma = \tfrac{1}{2}(N-2)[\tfrac{1}{2}(N-2)+1]$$

so that $\psi_o(N,1)$ is in fact an eigenstate of S^2, which we expect since $[S^2, \mathcal{H}_I] = 0$.

Recalling that $[S^-, S^2] = 0$ it is then clear that

$$S^2\psi_1(N,1) = \gamma\,\psi_1(N,1)$$

Repeated operation by S^- yields

$$S^2\,\psi_h(N,1) = \gamma\,\psi_h(N,1)$$

provided $h \leq N-2$. If we try to carry this process beyond $h = N-2$ there results,

$$S^2\,S^-\,\psi_{N-2}(N,1) =$$

$$S^2\,S^-[(N-2)!] \sum_{\substack{\ell=1 \\ \ell\neq j}}^{N}\sum_{j=1}^{N} e^{ikj}\,\beta_1\,\beta_2 \cdots \beta_{\ell-1}\,\alpha_\ell\,\beta_{\ell+1} \cdots \beta_j \cdots \beta_N =$$

$$S^2\,[(N-1)!]\,\Big(\sum_{j=1}^{N} e^{ikj}\Big)\,\beta_1\,\beta_2 \cdots \beta_N = 0\,,$$ which illustrates state-two above.

It is now clear that the interpretation that may be placed on $\psi_h(N,1)$ is that it represents a state having the same magnitude of spin, i, e., the same magnitude of magnetization, as the state represented by $\psi_o(N,1)$ but is tipped at an angle with respect to it.

These results just obtained for the case that started out with just one inversion present hold equally well for the two and three dimensional cases. But rather than proceed further with this restricted case the general validity of the two statements is assumed and the

partition function is calculated. Accordingly, the final results obtained at the end depend on the demonstration of the correctness of the statements when many inversions associated with $k \neq 0$ are present but should be valid if only one is present, i. e., they should be valid in the limit of low temperatures.

Making use of the fact that $[\mathcal{H}_I, S^-] = 0$, there results

$$\mathcal{H}_I \psi_h(H, r) = \mathcal{H}_I (S^-)^h \psi_o(N, r) = 2J \sum_{\nu=1}^{r} (1 - \cos k_\nu) \psi_h(N, r)$$

in which, using statement 1, none of the k's are zero and in which, using statement 2, $0 \leq h \leq N - 2r$. Thus it is seen that the h inversions do not contribute to the eigenvalue of $\mathcal{H}_I$.

We now have

$$\mathcal{H} \psi_h(N, r) = \left\{ 2J \sum_{\nu=1}^{r} (1 - \cos k_\nu) - \tfrac{1}{2} g\beta H(N - 2r - 2h) \right\} \psi_h(N, r)$$

so that the partition function is

$$Z = \sum_{r=0}^{\frac{1}{2}N} \sum_{k_1 \ldots k_r} \sum_{h=0}^{N-2r} \exp \left\{ \frac{1}{\kappa T} \left[-2J \sum_{\nu=1}^{r} (1 - \cos k_\nu) + \right. \right.$$

$$\left. \left. \tfrac{1}{2} g\beta HN - g\beta Hr - g\beta Hh \right] \right\}$$

or

$$Z = e^{\frac{g\beta HN}{2\kappa T}} \left[1 - e^{-\frac{g\beta H}{\kappa T}} \right]^{-1} Z'(H) + e^{-\frac{g\beta HN}{2\kappa T}} \left[1 - e^{\frac{g\beta H}{\kappa T}} \right]^{-1} Z'(-H) \quad (7)$$

where

$$Z'(H) = \sum_{r=0}^{\frac{1}{2}N} \sum_{k_1 \ldots k_r} \exp \left\{ -\frac{1}{\kappa T} \left[2J \sum_{\nu=1}^{r} (1 - \cos k_\nu) + g\beta Hr \right] \right\} \quad (8)$$

in which none of the k's are zero.

At this point it may be noted that when H is replaced by -H, Z is left unaltered so that M(N, T, -H) simply becomes -M(N, T, H) as is expected on physical grounds.

We may now observe that for sufficiently low T the terms for $r \neq 0$ can be neglected, so that

$$\lim_{T \to 0} Z'(H) \to \lim_{T \to 0} Z'(-H) \to 1$$

in all dimensionalities. This is because all $k = 0$ modes are excluded from Z' so that for $r \geq 1$

$$\lim_{T \to 0} \frac{1}{\kappa T} \left[2J \sum_{\nu=1}^{r} (1 - \cos k_\nu) + g\beta Hr \right] \to \infty$$

for any H. Then for finite H,

$$\lim_{T \to 0} Z \to e^{\frac{g\beta HN}{2\kappa T}}$$

so according to (5)

$$M(N, O, H) = \tfrac{1}{2} g\beta N$$

which shows no dependence on dimensionality. On the other hand, for finite but very low T (so that $Z'(H) \to 1$) there results

$$M(N, T, O) = O,$$

which again shows no dependence on dimensionality. These results are made more explicit in the following paragraphs.

Expanding the exponentials in powers of $\frac{g\beta H}{\kappa T}$ that appear in Z we obtain

$$Z = (N+1)Q_o - 2Q_1 + \left[\frac{N(N+1)(N+2)}{24} Q_o - \frac{(3N^2+6N+2)}{12} Q_1 + \frac{(N+1)}{2} Q_2 - \frac{1}{3} Q_3\right]\left(\frac{g\beta H}{\kappa T}\right)^2 + \left[\frac{N}{48}\left(\frac{N^4}{40} + \frac{N^3}{8} + \frac{N^2}{6} - \frac{1}{15}\right) Q_o - \frac{1}{8}\left(\frac{N^4}{24} + \frac{N^3}{6} + \frac{N^2}{6} - \frac{1}{45}\right) Q_1 + \frac{N}{8}\left(\frac{N^2}{6} + \frac{N}{2} + \frac{1}{3}\right) Q_2 - \frac{1}{12}\left(\frac{N^2}{2} + N + \frac{1}{3}\right) Q_3 + \frac{(N+1)}{24} Q_4 - \frac{1}{60} Q_5\right]\left(\frac{g\beta H}{\kappa T}\right)^4 + \cdots \tag{9}$$

in which

$$Q_\ell = \sum_{r=0}^{\frac{1}{2}N} \sum_{k_1 \cdots k_r} r^\ell \exp\left\{-\frac{2J}{\kappa T} \sum_{\nu=1}^{r}{}' (1 - \cos k_\nu)\right\} \tag{10}$$

Thus for small H (the criterion for "small" is given below)

$$\frac{M(N, T, H)}{M_o} \cong \frac{\frac{1}{6}(N+1)(N+2) Q_o - \frac{1}{3}(3N + 6 + \frac{2}{N}) Q_1 + (1 + \frac{1}{N}) Q_2 - \frac{4}{3N} Q_3}{(N+1)Q_o - 2Q_1} \cdot \frac{g\beta H}{\kappa T} \tag{11}$$

in which $M_o = \frac{1}{2} g \beta N$. For finite temperatures, it is clear that the Q's are all finite and, therefore, the magnetization is finite or zero in any dimensionality if the applied field is respectively finite or zero. This result shows that there is no essential dependence of magnetization on dimensionality in the sense that the condition required to make it vanish in any dimension is sufficient to make it vanish in all dimensions, and the condition required to make it finite in any dimension is sufficient to make it finite in all dimensions. The actual value of the relative magnetization will, of course, depend on the dimensionality in the finite case.

If one assumes T small enough to insure $\frac{2J}{\kappa T} \gg 1$ so that on the average $r \ll N$, implying a temperature much lower than the Curie temperature, then it can be seen from equation (10) that

$$N Q_\ell \gg Q_{\ell+1}$$

Making use of this condition and also the usual situation of $N \gg 1$, equation (9) becomes

$$Z \cong N Q_o \left[1 + \frac{1}{24} \left(\frac{g \beta H N}{\kappa T} \right)^2 + \frac{1}{1920} \left(\frac{g \beta H N}{\kappa T} \right)^4 \right] \qquad (12)$$

which shows that the criterion for small H is that $\frac{g \beta H N}{\kappa T} \ll 1$. Under these conditions

$$\frac{M(N, T, H)}{M_o} \cong \frac{1}{6} \frac{g \beta H N}{\kappa T} \qquad (13)$$

That is, for sufficiently small H the magnetization is independent of the strength of the interaction between the spins.

On the other hand, it can be seen that for large $\frac{g \beta H N}{\kappa T}$ and for

small enough T to insure on the average $r << N$ the second term of equation (7) may be neglected compared to the first. In this case,

$$\frac{M(N, T, H)}{M_o} \cong 1 + \frac{\kappa T}{M_o} \frac{\partial \ln Z'(H)}{\partial H} - \frac{2}{N}\left[1 - \exp\left(-\frac{g\beta H}{\kappa T}\right)\right]^{-1}$$

or, approximating the sum on k_ν by an integral[5, 6, 7] and neglecting the last term,

$$\frac{M(N, T, H)}{M_o} \cong 1 - \frac{p}{(2\pi)^D} \int_{\frac{2\pi}{G}}^{\infty} k^{D-1}\left[e^{\frac{Jk^2}{\kappa T}} e^{\frac{g\beta H}{\kappa T}} - 1\right]^{-1} dk \quad (14)$$

where $p = 1, 2\pi, 4\pi$ according as $D = 1, 2, 3$. D is the dimensionality of the single domain sample, and G is the length of the linear chain or is the length of an edge in the two or three dimensional cases measured in units of lattice spacing, i.e., $G^D = N$.

Equation (14) should be used with some caution. It must be remembered that $\frac{g\beta HN}{\kappa T} >> 1$ is required. This ordinarily does not place much restriction on H in the three dimensional case unless one is dealing with small numbers of particles. Also in the three dimensional case it is customary to evaluate the integral for the case $H = 0$ and with the lower limit zero instead of $\frac{2\pi}{G}$, since there is not much contribution to the integral near the origin. This procedure gives results for $M(N, T, O)/M_o \sim 1$ while equation (13) predicts an answer of zero. This discrepancy is due to the fact that (14) is a very crude approximation to $\kappa T \frac{\partial \ln Z}{\partial H}$ for very small H, i.e., $H << \frac{\kappa T}{g\beta N}$. However, it should be emphasized that there is no disagreement with the numerical results of (14) that are usually quoted since for such results it is assumed that

at least a very small H exists--and once this is granted, (14) is very nearly independent of H over an enormous range and nearly equals the values obtained from (14) for the case H = 0.

In the two dimensional case the mathematical reduction of (14) can be carried further, yielding, after integration,

$$\frac{M(N, T, H)}{M_o} = 1 - \frac{\kappa T}{4\pi J} \ln \left[1 - e^{-\frac{g\beta H}{\kappa T}} e^{-\frac{4\pi^2 J}{N\kappa T}} \right]^{-1}. \qquad (15)$$

A wide range of physical interest is included if the parameters are restricted to the intervals

$$10^3 °K > T > 10 °K,$$
$$10^4 Oe > H > .1 \text{ Oe},$$
$$N > 10^9.$$

Such restrictions insure $\frac{g\beta HN}{\kappa T} >> 1$ so that (15) is valid provided the resulting value for $M(N, T, H)/M_o$ is near one. Such restrictions also make $\frac{g\beta H}{\kappa T} >> 1$. Equation (15) then, for very large N, reduces to

$$\frac{M(N, T, H)}{M_o} = 1 - \frac{\kappa T}{4\pi J} \ln \left(\frac{\kappa T}{g\beta H} \right).$$

3. Conclusions

It has been established, with the help of several statements that are not proved herein, that the behavior of a magnetic system has no essential dependence on dimensionality. Equation (13) shows that for sufficiently low fields the relative magnetization is independent of the interaction between spins. For high fields the results, summarized in equation (14), are of the same form as previously obtained. The important difference is that the existance of a finite lower limit on the integral has been demonstrated, which, together with a finite H assures one of a finite temperature range in which ferromagnetism will occur.

It appears that there exist a range of parameters, J, N, and H (for low T) that produce results between those of equations (13) and (14) that would be of experimental interest. The possibility of the numerical reduction of the formulas in these cases is currently under investigation.

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