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# Removal of an Apparent Discrepancy between Calculations of Dyson and of Oguchi for the Heisenberg Ferromagnet

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An apparent discrepancy between the published results of Dyson and of Oguchi for the coefficient of the $T^4$ term in the low-temperature magnetization of a simple cubic ferromagnet is shown to result from the different numerical approximations used by these authors. The coefficient correct to 5 figures is shown to include a factor $\{1+0.29562/S+0(1/S^2)+\cdots\}$.

## 1. INTRODUCTION

THE purpose of this paper is to remove an apparent discrepancy[1] between the published results of the boson approximation to the low-temperature behavior of the simple cubic Heisenberg ferromagnet as calculated by Dyson[2] and by Oguchi.[3]

The discrepancy appears in the coefficient of the lowest order spin-wave-interaction contribution to the magnetization $M(T)$, the $T^4$ term. Dyson's result contains a numerical factor when expanded and retained to order $1/S$ of

$$\{1+0.31/S+0(1/S^2)+\cdots\}, \qquad (1)$$

whereas Oguchi's, calculated only to this order, gives for the same factor

$$\{1+0.2/S+0(1/S^2)+\cdots\}. \qquad (2)$$

Despite the practical insignificance of this discrepancy and despite the formal equivalence of the boson models used by these authors this discrepancy appears to have left doubts in the minds of a number of authors as to the consistency of these models.

We show how the calculations of both Dyson and Oguchi for the coefficient may be reduced to identical analytical expressions. The discrepancy results merely from the different numerical approximations they used to evaluate the integrals (see Table I). The answer correct to 5 significant figures turns out to be

$$\{1+0.29562/S+0(1/S^2)+\cdots\}. \qquad (3)$$

## 2. THE BOSON APPROXIMATION

Dyson's boson model for the Heisenberg ferromagnet is obtained by using the Maleev[4] substitution for the spin operators which in the spin-wave representation gives (using Dyson's notation with 1, 2, etc. standing for $k_1$, $k_2$, etc.)

$$H_{\rm Dy}=\sum_k (L+\epsilon_k)a_k^\dagger a_k +\left(\frac{J}{2N}\right)\sum_{1,2,3}(\gamma_1-\gamma_{1-3})a_1^\dagger a_2^\dagger a_3 a_{1+2-3} \qquad (4)$$

As Dyson and, more recently, Wortis[5] showed, the non-Hermitian character of Eq. (4) and the use of Bose statistics leads to improper states with an unphysical number of spin deviations which must be removed by kinematic corrections. However, these corrections have been shown by Dyson[2] and by Wortis[5] to be certainly negligible at low temperatures.

Oguchi worked with the Holstein-Primakoff (HP) substitution which he expanded in powers of $1/S$ to obtain, in notation as in Eq. (4),

$$H_{\rm Og}=\sum_k (L+\epsilon\ )a_k^\dagger a_k +\left(\frac{J}{4N}\right)\sum_{1,2,3}\left\{(\gamma_1+\gamma_2)\left(1+\frac{1}{8S}+\cdots\right)-2\gamma_{2-4}\right\} \times a_1^\dagger a_2^\dagger a_3 a_{1+2-3}+\cdots. \qquad (5)$$

Oguchi showed that his Hamiltonian is equivalent to Dyson's to at least order $1/S$. Oguchi, Morkowski, and Dembinski[6] have since pointed out that the Maleev substitution may be generally connected with that of HP by a similarity transformation.

Thus for temperatures low enough for the contributions from the improper eigenvalues resulting from Eqs. (4) and (5) and their associated kinematic corrections to be negligible, the two models must give identical results to all orders in $1/S$.

## 3. THE $T^4$ TERM

Oguchi proceeded to calculate the free energy by perturbation theory using Eq. (5) to second order in the spin-wave interaction. In fact the results he obtained are analytically identical to those obtained by Dyson, as must result from the equivalence of the Hamiltonians

[1] See for instance L. R. Walker in *Magnetism*, edited by G. T. Rado and H. Suhl (Academic Press Inc., New York, 1963), Vol. 1, Chap. 8.
[2] F. J. Dyson, Phys. Rev. **102**, 1217 (1956); **102**, 1230 (1956).
[3] T. Oguchi, Phys. Rev. **117**, 117 (1960).
[4] S. V. Maleev, Zh. Eksperim. i Teor. Fiz. **33**, 1010 (1957) [English transl.: Soviet Phys.—JETP **6**, 776 (1958)]. See also G. Avakiants, Zh. Eksperim. i Teor. Fiz. **18**, 444 (1948).
[5] M. Wortis, Phys. Rev. **138**, A1126 (1965).
[6] T. Oguchi, Progr. Theoret. Phys. (Kyoto) **25**, 721 (1961); J. Morkowski, *ibid.* **27**, 1284 (1962); S. T. Dembinski, Physica **30**, 1217 (1964).

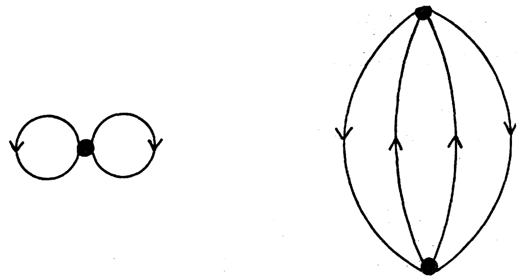

FIG. 1. Lowest order diagrams contributing to the free energy.

to order $1/S$ as mentioned above. However, the numerical discrepancy obscured this equivalence at the time.

An equivalent calculation starting from Dyson's Hamiltonian, Eq. (4), has been given by Szczeniowski *et al.*,[7] (S.M.S.) using a diagram expansion for the free energy.[8] As has been shown by Dyson, Oguchi, and S. M. S., only those perturbation contributions that are described by the diagrams in Fig. 1 contribute to the orders of $T$ and $1/S$ in which the discrepancy occurs.

The calculations from the diagrams in Fig. 1 using the Hamiltonian, Eq. (4), have been shown by Szaniecki[9] to lead to the same contribution to the magnetization, expanded to order $1/S$, as that quoted by Dyson, namely, a factor

$$\{1+[(2\Gamma+\alpha)/3]1/S+0(1/S^2)+\cdots\}, \qquad (6)$$

where, for the simple cube,

$$\Gamma=\frac{3}{(2\pi)^3}\int_{-\pi}^{+\pi}d^3X\frac{\cos X(1-\cos Y)}{3-\sum_i \cos X_i}, \qquad (7)$$

and

$$\alpha=-1+\frac{3}{(2\pi)^3}\int_{-\pi}^{+\pi}d^3X\frac{1}{3-\sum_i \cos X_i}. \qquad (8)$$

On the other hand, starting from the Hamiltonian, Eq. (5), the contributions to the free energy from Fig. 1 may be shown to be identical to those derived by Oguchi. These lead to a factor which Oguchi did not give explicitly, but which may be derived from his Eq. (21) as

$$\{1+\Delta/S+0(1/S^2)+\cdots\}, \qquad (9)$$

where

$$\Delta=\frac{2}{(2\pi)^3}\int_{-\pi}^{+\pi}d^3X\frac{\cos^2 X}{3-\sum_i \cos X_i}. \qquad (10)$$

Inspection of the integrands in Eqs. (7), (8) and (10), using the identity

$$\frac{\cos X}{3-\sum_i \cos X_i}=-1+\frac{3-\cos Y-\cos Z}{3-\sum_i \cos X_i}, \qquad (11)$$

shows that

$$\Delta=(2\Gamma+\alpha)/3 \qquad (12)$$

and so Eqs. (6) and (9) are analytically equal.[7]

## 4. NUMERICAL EVALUATION

Dyson used an accurate evaluation of $\alpha$ in terms of complete elliptic functions by Watson,[10] giving

$$\alpha=0.516368, \qquad (13)$$

and an approximate numerical evaluation of

$$\Gamma\approx\tfrac{1}{5}, \qquad (14)$$

to obtain

$$(2\Gamma+\alpha)/3=0.31. \qquad (15)$$

Oguchi did not state explicitly his method of evaluation, but we have retrieved his expansion by rewriting Eq. (10) as a Laplace transform of a product of modified Bessel functions, using the integral representation

$$I_\nu(u)=\frac{1}{2\pi}\int_{-\pi}^{+\pi}e^{u\cos x}\cos\nu x\,dx \qquad (16)$$

to obtain

$$\Delta=4\pi^3\int_0^\infty du\,e^{-3u}I_0^2(u)\{I_0(u)+I_2(u)\}. \qquad (17)$$

Oguchi's approximation is obtained by expanding $I_\nu(u)$ in powers of $u$ from which one finds[11]

$$\Delta=\tfrac{1}{6}+7/216+\cdots\approx 0.2+\cdots. \qquad (18)$$

However, this series converges extremely slowly, thus explaining the inaccuracy of Oguchi's approximation.

More accurate values of $\Delta=(2\Gamma+\alpha)/3$ can be obtained from related integrals which have been obtained numerically in other connections by Slater and Koster.[12] Wolfram and Callaway[13] got the same results as the latter by a similar method using Simpson's rule in steps of 0.01 from $u=0$ to 50 and thus obtained larger than correct contributions from this range while neglecting the contributions from larger values. From these values we get $\Delta$ or $(2\Gamma+\alpha)/3$ to an accuracy of a few percent (see Table I).

A more accurate method is to use the power series for small $u$ together with an asymptotic expansion of the $I_\nu(u)$ for large $u$. This method was used by Maradudin *et al.*,[14] from which the value, correct to 5 significant figures of

$$(1+0.29562/S+\cdots) \qquad (19)$$

is obtained.

[7] S. Szczeniowski, J. Morkowski and J. Szaniecki, Phys. Status Solidi 3, 537 (1963).
[8] T. Matsubara, Progr. Theoret. Phys. (Kyoto) 14, 351 (1955); J. M. Luttinger and J. C. Ward, Phys. Rev. 118, 1417 (1960).
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[13] T. Wolfram and J. Callaway, Phys. Rev. 130, 2207 (1963).
[14] A. A. Maradudin, E. W. Montroll, G. H. Weiss, R. Herman and E. W. Milnes, Acad. Roy. Belge, Classe Sci. Mem. 14, No. 1709 (1960).

TABLE I. Numerical values of the integrals in Eqs. (7) and (8).

| | $\Gamma$ | $\alpha$ | $\frac{2\Gamma+\alpha}{3}$ | $\Delta$ |
|---|---|---|---|---|
| Dyson[a] | $\frac{1}{6}$ | 0.516386[b] | 0.31 | ... |
| Oguchi[c] | ... | ... | ... | 0.2 |
| Wolfram and Callaway[d] and Table III of Slater and Koster[e] | 0.2598[f] | 0.4778[f] | 0.332[f] | 0.295[f,g] |
| Table I of Slater and Koster[e] | ... | ... | ... | 0.288[f] |
| Maradudin *et al.*[h] | 0.185238[f] | 0.516386[f,i] | 0.29562[f] | 0.29562[f] |

[a] Reference 2.
[b] Watson's value.
[c] Reference 3.
[d] Reference 13.
[e] Reference 12.
[f] Compounded from related integrals.
[g] This is near the correct value because of cancellation of errors between the integrals from which it is compounded.
[h] Reference 14.
[i] Equal to Watson's value.

We thus conclude that for temperatures below those for which kinematic corrections are important (Wortis[5] gives a rough estimate that they will only be so in the $T^{(3/2)(2S+1)^4}$ term for a 3-dimensional ferromagnet, i.e., the $T^{24}$ term for $S=\frac{1}{2}$, and even higher for larger spins) there is no evidence of any inconsistency between the boson models used by Dyson and by Oguchi. In practice Dyson's Hamiltonian is much the simpler to use as it involves only spin-wave pair interactions. Thus it enabled Dyson to sum the infinite series of ladder diagrams contributing to the $T^4$ term to give its exact dependence on $S$, whereas this would be exceedingly difficult using the Holstein-Primakoff method because of the need to cancel contributions between various orders of perturbation theory. This cancellation was shown to occur between contributions from the two graphs of Fig. 1 to order $1/S$ by Oguchi, but has not been demonstrated generally.

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# Spin-Spin Relaxation in $LaF_3$†

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The present work is a study by nmr pulse techniques of the motion of fluorine atoms in lanthanum trifluoride as a function of temperature, between 100 and 560°C. The experiments have been conducted with a single crystal of $LaF_3$. The model for the motions derived from this study is the following: There are two types of fluorine nuclei, the spins $I$ and the spins $S$, located on different sublattices. Between 100 and 300°C, the motion of the spins $I$ is fast (i.e., such as to be appreciable in times shorter than the reciprocal of the rigid-lattice line width), and the motion of the spins $S$ is slow. There is an exchange of atoms between the two sublattices, the rate of which is slow up to about 300°C and fast at higher temperature. The ratio of populations of the spins $I$ and $S$ is $N_I/N_S=2$. Approximate values are derived for the activiation energies associated with these two types of motion.

## I. INTRODUCTION

NUCLEAR magnetic resonance is a well-established tool for the study of motions in solids; detailed descriptions of its use in this respect, together with references to early works, can be found in general textbooks.[1–4] Its use is based on the fact that the averaging of spin-spin interactions between nuclei by atomic motions profoundly affects the line width and the spin-lattice relaxation of nuclear spin systems, as soon as the rate of change of the spin-spin interactions is faster than the static linewidth, typically a few kcps, although the method has been recently extended[5,6] to far lower rate values by the measurement of the spin-lattice relaxation time of the spin-spin interactions.

The present work consists of a study of the fluorine spin-spin relaxation in lanthanum trifluoride between 100 and 560°C, in a temperature range where atomic motions have a dominant influence on this relaxation. In a recent study[7] of the fluorine line shape in this com-

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