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Spin Waves in an Antiferromagnet with $S=\frac{1}{2}$†

J. Korringa
Department of Physics, The Ohio State University, Columbus, Ohio
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It is shown that of two conflicting corrections to the dispersion law for spin waves in an antiferromagnetic, Fu-Cho Pu's is rather accurate for short waves, whereas Oguchi's is quite good for long waves. The operator method in terms of spin-flip operators is used in first and second approximation.

1. INTRODUCTION

THE spectrum of spin-wave excitations in an antiferromagnet with $S=\frac{1}{2}$ has recently been given in two different approximate forms. Fu-Cho Pu[1] derived the expression

$$\mathcal{E}_p=E_p-E_0=z(1-2\Delta)(1-\gamma_p^2)^{\frac{1}{2}}, \tag{1}$$

which differs by the factor $(1-2\Delta)$ from the result found much earlier by Anderson.[2] Oguchi,[3] on the other hand, obtained

$$\mathcal{E}_p=z(1+\sigma)(1-\gamma_p^2)^{\frac{1}{2}}, \tag{2}$$

where σ, like Δ, is a positive constant.

Equations (1) and (2) apply to an isotropic spin Hamiltonian. The exchange interaction J between nearest neighbors is used as unit of energy. z is the number of nearest neighbors. γ_p is given by

$$\gamma_p=(1/z)\textstyle\sum_\delta \exp(i\boldsymbol{\delta}\cdot\mathbf{p}), \tag{3}$$

summed over nearest neighbor vectors $\boldsymbol{\delta}$. The constant Δ in Eq. (1) is equal to the deviation from perfect alignment of the spins of each sublattice, existing in the ground state. As was shown in reference 1, Δ is of the form:

$$\Delta=\tau/(1+2\tau), \tag{4}$$

where

$$\tau=\tfrac{1}{2}(1/N)\textstyle\sum_p[(1-\gamma_p^2)^{-\frac{1}{2}}-1]. \tag{5}$$

The constant σ in Eq. (2) is given by

$$\sigma=(1/N)\textstyle\sum_p[1-(1-\gamma_p^2)^{\frac{1}{2}}]. \tag{6}$$

The numerical values of τ and σ for the 2-dimensional square lattice and for the 3-dimensional simple-cubic and body-centered cubic lattices were already calculated by Anderson and Kubo.[4]

Fu-Cho Pu obtained his result in the representation of spin-flip operators with Greens' function methods, by evaluating 2-spin Greens' functions while truncating those for four spins. Oguchi used the representation of Primakoff and Holstein, by expanding their spin deviation operators up to and including terms in $1/S$ and performing a canonical transformation to bring out the elementary excitations.

In order to investigate the source of the discrepancy between Eqs. (1) and (2), I have used a method in which one constructs explicitly the operators $\mathcal{O}_p^\dagger$ and $\mathcal{O}_p$ which create and annihilate spin wave excitations, in terms of the spin-flip operators $a_j^\dagger$ and a_j. The convenience of this method—which is equivalent to Fu-Cho Pu's approach—is well illustrated by Suhl and Werthamer's treatment of the electron gas.[5] In Sec. 2 it will be shown that Eqs. (1), (4), and (5) are obtained by restricting $\mathcal{O}_p^\dagger$ and $\mathcal{O}_p$ to linear expressions in $a_j^\dagger$ and a_j. An extension to include trilinear terms is given in Sec. 3. In Sec. 4 some numerical results are discussed in relation to the differences between Eqs. (1) and (2).

2. LINEAR APPROXIMATION

In terms of the spin-flip operators of lattice site j, $x_j=(a_j^\dagger \text{ or } a_j)$, which are defined as usual,[6] the Hamiltonian takes the form:

$$H=z\textstyle\sum_j a_j^\dagger a_j+\frac{1}{2}\sum_{j\delta}(a_j^\dagger a_{j+\delta}^\dagger+a_ja_{j+\delta}) -\sum_{j\delta}a_j^\dagger a_j a_{j+\delta}^\dagger a_{j+\delta}, \tag{7}$$

with

$$\begin{aligned}&[x_j,x_k]_-=0, \quad (j\neq k)\\ &[a_j^\dagger,a_j]_+=1, \quad x_j^2=0.\end{aligned} \tag{8}$$

Let a spin-wave excitation with energy E_p be created by operating with $\mathcal{O}_p^\dagger$ on the ground state ψ_0. This gives:

$$H\mathcal{O}_p^\dagger\psi_0=E_p\mathcal{O}_p^\dagger\psi_0 \tag{9}$$

or

$$([H,\mathcal{O}_p^\dagger]_- -\mathcal{E}_p\mathcal{O}_p^\dagger)\psi_0=0, \tag{10}$$

In the linear approximation $\mathcal{O}_p^\dagger$ and the corresponding annihilation operator $\mathcal{O}_p$ take the form:

$$\mathcal{O}_p^\dagger=\alpha_+X_p^\dagger+\alpha_-X_p, \quad \mathcal{O}_p=\alpha_+X_p+\alpha_-X_p^\dagger, \tag{11}$$

with undetermined real p-dependent coefficients α_+ and α_-, where

$$\begin{aligned}X_p^\dagger&=(1/N)^{\frac{1}{2}}\textstyle\sum_j a_j^\dagger \exp(i\mathbf{p}\cdot\mathbf{j}),\\ X_p&=(1/N)^{\frac{1}{2}}\textstyle\sum_j a_j.\exp(-i\mathbf{p}\cdot\mathbf{j}).\end{aligned} \tag{12}$$

The commutator in Eq. (10) yields, besides linear terms,

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[1] Fu-Cho Pu, Soviet Phys. Doklady **5**, 128 (1960).

[2] P. W. Anderson, Phys. Rev. **86**, 694 (1952), see also J. M. Ziman, Proc. Roy. Soc. (London) **A65**, 540 and 548 (1952) and R. Kubo, Phys. Rev. **87**, 568 (1952).

[3] T. Oguchi, Phys. Rev. **117**, 117 (1960).

[4] See reference 2. $\tau=\frac{1}{2}c'$ and $\sigma=c$ in Oguchi's notation. Note that the sums (5) and (6) extend over the entire reciprocal lattice. Anderson has $\Delta=\tau$ instead of Eq. (4).

[5] H. Suhl and N. R. Werthamer, Phys. Rev. **122**, 359 (1961).

[6] R. L. Mills, R. P. Kenan, and J. Korringa, Physica **26**, S204 (1960).

cubic terms of the form $x_j a_{j+\delta}^\dagger a_{j+\delta}\psi_0$. These are replaced by $x_j\psi_0\Delta$, where $\Delta=\langle\psi_0|a_j^\dagger a_j|\psi_0\rangle$ is still to be determined. The resulting equation can be solved regardless of the form of ψ_0 by requiring that the operator $[H,\mathcal{O}_p^\dagger]_- - \mathcal{E}_p\mathcal{O}_p^\dagger$, which is now linear in the x_j, vanish identically.

This gives

$$\begin{aligned}(-\mathcal{E}_p/J'+z)\alpha_+ - z\gamma_p\alpha_- &= 0\\ z\gamma_p\alpha_+ - (\mathcal{E}_p/J'+z)\alpha_- &= 0,\end{aligned} \tag{13}$$

where $J'=1-2\Delta$, or

$$\mathcal{E}_p = z(1-2\Delta)(1-\gamma_p^2)^{\frac{1}{2}}, \tag{14}$$

as in Eq. (1) and

$$\alpha_+=\gamma_p, \quad \alpha_-=1-(1-\gamma_p^2)^{\frac{1}{2}}. \tag{15}$$

The self-consistency relation for determining Δ can be obtained as follows.[7] From Eq. (11) one has

$$X_p^\dagger = u_+\mathcal{O}_p^\dagger - u_-\mathcal{O}_p, \tag{16}$$

and conjugate, with

$$u_\pm = \alpha_\pm/(\alpha_+^2-\alpha_-^2). \tag{17}$$

Therefore

$$a_j^\dagger = (1/N)^{\frac{1}{2}}\sum_p(u_+\mathcal{O}_p^\dagger - u_-\mathcal{O}_p)\exp(-i\mathbf{p}\cdot\mathbf{j}), \tag{18}$$

and conjugate.

Consequently

$$\begin{aligned}\Delta=\langle a_j^\dagger a_j\rangle_0 = (1/N)\textstyle\sum_{pp'}\langle(u_+\mathcal{O}_p^\dagger - u_-\mathcal{O}_p)(u_+'\mathcal{O}_{p'}\\ -u_-'\mathcal{O}_{p'}^\dagger)\rangle_0 \exp[i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{j}].\end{aligned} \tag{19}$$

It is seen that with any pair $\mathcal{O}_{p'}^\dagger,\mathcal{O}_p^\dagger$, of approximate solutions of Eq. (10) as operator equation, their product is a solution with energy $\mathcal{E}_{p'}+\mathcal{E}_p$. This establishes these approximate excitations as Bosons. Consistency requires therefore that the ground state expectation value of products of $\mathcal{O}_p^\dagger$ and $\mathcal{O}_{p'}$ appearing in Eq. (19) are zero with the exception of $\langle\mathcal{O}_p\mathcal{O}_p^\dagger\rangle_0$. The value of $\langle\mathcal{O}_p\mathcal{O}_p^\dagger\rangle_0$ can be obtained from the commutator. Equations (11) and (12) give:

$$\begin{aligned}[\mathcal{O}_p,\mathcal{O}_p^\dagger]_- &= (\alpha_+^2-\alpha_-^2)[X_p,X_p^\dagger]_-\\ &= (1/N)(\alpha_+^2-\alpha_-^2)\textstyle\sum[a_j,a_j^\dagger]_-\end{aligned} \tag{20}$$

or

$$\langle[\mathcal{O}_p,\mathcal{O}_p^\dagger]_-\rangle_0 = \langle\mathcal{O}_p\mathcal{O}_p^\dagger\rangle_0 = (\alpha_+^2-\alpha_-^2)(1-2\Delta). \tag{21}$$

Inserting (21) in (19) gives:

$$\Delta=(1-2\Delta)(1/N)\textstyle\sum_p \alpha_-^2/(\alpha_+^2-\alpha_-^2). \tag{22}$$

Inserting the values of $\alpha_\pm$ from Eq (15) gives immediately Eqs. (4) and (5).

3. CUBIC APPROXIMATION

The next approximation is obtained by including in $\mathcal{O}_p^\dagger$ the following trilinear terms in the x_j, with coefficients that have to be determined:

1. The terms $x_j a_{j+\delta}^\dagger a_{j+\delta}$, which appear in $[H,x_j]_-$ and which were linearized in the linear approximation.
2. Those terms $x_j x_{j+\delta} x_{j+\delta'}$ ($\delta\neq\delta'\neq 0$) which appear in $[H,x_j a_{j+\delta}^\dagger a_{j+\delta}]_-$.

Not to be included are *disconnected* trilinear terms, which appear in $[H,x_j x_{j+\delta} x_{j+\delta'}]_-$. In fifth-order terms of the form $x_j x_{j+\delta} x_{j+\delta'} a_k^\dagger a_k$, which appear in this same commutator, the factor $a_k^\dagger a_k$ is to be replaced by Δ; all other fifth-order terms are to be discarded.

With these approximations, Eq. (10) can again be solved as an operator equation. The number of unknown coefficients is large because the coefficient of a term $x_j x_{j+\delta} x_{j+\delta'}$ depends on its orientation with respect to $\mathbf{p}$. The result is:

$$\begin{aligned}\mathcal{O}_p^\dagger = &\textstyle\sum_j(\alpha_j^+ a_j^\dagger + \alpha_j^- a_j) + \sum_{j\delta}(\beta_{j\delta}^+ a_j^\dagger a_j a_{j+\delta}^\dagger\\ &+\beta_{j\delta}^- a_j^\dagger a_j a_{j+\delta}) + \textstyle\sum_{j\delta\delta'}(\frac{1}{2}\gamma_{j\delta\delta'}^3 a_j^\dagger a_{j+\delta}^\dagger a_{j+\delta'}^\dagger\\ &+\gamma_{j\delta\delta'}^1 a_j^\dagger a_{j+\delta}^\dagger a_{j+\delta'} + \gamma_{j\delta\delta'}^{-1} a_j a_{j+\delta} a_{j+\delta'}^\dagger\\ &+\tfrac{1}{2}\gamma_{j\delta\delta'}^{-3} a_j a_{j+\delta} a_{j+\delta'}),\end{aligned} \tag{23}$$

where

$$\begin{aligned}0=(\mathcal{E}\mp z)\alpha_j^\pm \pm \textstyle\sum_\delta \alpha_{j-\delta}^\mp \pm \frac{1}{2}\xi\sum_\delta \beta_{j\delta}^\mp\\ \mp(1-\Delta)\textstyle\sum_{\delta\delta'}(\gamma_{j-\delta,\delta,\delta'}^{\pm 3} - \gamma_{j-\delta',\delta,\delta'}^{\mp 1}),\end{aligned} \tag{24a}$$

$$\begin{aligned}0=(\mathcal{E}\mp z\pm\xi)\beta_{j\delta}^\pm \pm 2\alpha_{j+\delta}^\pm \mp 2\alpha_j^\mp \mp (\xi-1)\beta_{j+\delta,\delta}^\mp\\ \pm\textstyle\sum_{\delta'}(\gamma_{j\delta\delta'}^{\pm 3} - \gamma_{j\delta'\delta}^{\mp 1}),\end{aligned} \tag{24b}$$

$$\begin{aligned}0=(\mathcal{E}\mp a)\gamma_{j\delta\delta'}^{\pm 3} \pm \beta_{j\delta}^\pm \pm \beta_{j\delta'}^\pm\\ \pm(1-2\Delta)(\gamma_{j+\delta,-\delta,\delta'}^{\pm 1} + \gamma_{j+\delta',-\delta',\delta}^{\pm 1}),\end{aligned} \tag{24c}$$

$$\begin{aligned}0=(\mathcal{E}\mp b)\gamma_{j\delta\delta'}^{\pm 1} \pm \beta_{j\delta'}^\mp\\ \mp(1-2\Delta)(\gamma_{j+\delta,-\delta,\delta'}^{\pm 3} - \gamma_{j+\delta',\delta,-\delta'}^{\mp 1}),\end{aligned} \tag{24d}$$

with

$$\begin{aligned}\xi&=2+2(z-1)\Delta,\\ a&=(3z-4)(1-2\Delta),\\ b&=(z-2)(1-2\Delta).\end{aligned} \tag{24e}$$

By summing Eqs. (b) over δ, Eqs. (c) and (d) over δ and δ' with $\delta+\delta'\neq 0$ and separately over δ with $\delta+\delta'=0$, and by performing a Fourier transformation one obtains 12 equations with 12 unknowns; the two resulting groups of terms in γ^i correspond to geometrically inequivalent configurations. The corresponding eigenvalue equation for $\mathcal{E}_p$—written as $\mathcal{E}$ for simplicity—can be cast in the following form:

$$\begin{vmatrix}\mathcal{E}/z & -\gamma-1 & 2\mathcal{E}A\gamma(1-\Delta) & -\xi+2B_+\gamma(1-\Delta)\\ \gamma-1 & \mathcal{E}/z & \xi+2B_-\gamma(1-\Delta) & 2\mathcal{E}A\gamma(1-\Delta)\\ 0 & \gamma+1 & \mathcal{E}(1-A) & -\gamma(1-\xi)+\xi-z-B_+\\ \gamma-1 & 0 & \gamma(1-\xi)+\xi-z-B_- & \mathcal{E}(1-A)\end{vmatrix}=0, \tag{25}$$

[7] This was suggested to me by R. L. Mills and A. M. Sessler during a seminar discussion.

where γ is given by Eq. (3) and where

$$A=(3\mathcal{E}^2-a^2-2b^2)[(z-2)D^{-1}+D_0^{-1}]+4c^2(z-2)D^{-1},$$

$$B_\pm=[\mathcal{E}^2(2a-b)+ab(a-2b)][(z-2)D^{-1}+D_0^{-1}]\pm c[5\mathcal{E}^2+a(4b-a)+4c^2\mp 4bc](z-2)D^{-1}, \tag{26}$$

$$c=\gamma(1-2\Delta),$$

$$D=[(\mathcal{E}-a)(\mathcal{E}-b)+2c^2][(\mathcal{E}+a)(\mathcal{E}+b)+2c^2]+c^2(\mathcal{E}^2-a^2), \tag{27}$$

$$D_0=D(c=0).$$

Equation (25) is even in $\mathcal{E}$. As is seen from Eq. (10), the negative roots correspond to the annihilation operators $\mathcal{O}_p$, which are the Hermitian conjugate of $\mathcal{O}_p^\dagger$. It can also be seen that Eq. (25) is even in γ, thus preserving the degeneracy of bands which is manifest in the linear approximation.

A selfconsistent determination of Δ with a method similar to that of Sec. 2 can only be carried out with elaborate and purely numerical calculations. Instead, its value in the linear approximation will be used.

4. NUMERICAL RESULTS AND DISCUSSION

A root of Eq. (25) has been determined in the limit of long wavelength for which $(1-\gamma)$ is a small quantity, and for those (short) wavelengths for which $\gamma=0$. In the former case one expects $\mathcal{E}^2\propto 1-\gamma$. Retaining in Eq. (25) only terms in $\mathcal{E}^0$ and $\mathcal{E}^2$ one finds

$$\mathcal{E}=(1+K)z(1-\gamma^2)^{\frac{1}{2}}. \tag{28}$$

The value of K for $z=4$, 6, and 8 was obtained while using Δ from Eq. (4) with Anderson's values of τ. These are listed in Table I under the heading K_Δ. A calculation with $\Delta=0$ was performed, and is listed under K_0, in order to show the influence of fifth order terms in their approximate form as discussed in Sec. 3. It should be noted that in the trilinear terms $x_j a_{j+\delta}^\dagger a_{j+\delta}$, $a^\dagger a$ has not been replaced by Δ.

For $\gamma=0$ one expects from Eq. (1) $\mathcal{E}\propto z(1-2\Delta)$. The quantity

$$Y=\mathcal{E}/z-1+2\Delta, \tag{29}$$

TABLE I. Energy in the long wavelength limit in terms of K, defined by Eq. (28).

z	τ[a]	Δ[b]	K_Δ	K_0	K_1[c]
4	0.197	0.141	−0.13	0.51	...
6	0.078	0.068	+0.20	0.34	0.194
8	0.075	0.064	+0.16	0.25	0.146

[a] From reference 2. [b] From Eq. (4). [c] From Eq. (2).

TABLE II. Energy for short waves with $\gamma=0$ in terms of Y, defined by Eq. (29).

z	Y_Δ	Y_0	Y_1[b]
4	−0.092	+0.14	...
6	−0.017	...[a]	0.28
8	+0.037	+0.05	0.25

[a] No real roots exist for this case. [b] From Eq. (2).

has been calculated with the value of Δ from Eq. (4) and also for $\Delta=0$. The results are given in Table II under the heading Y_Δ and Y_0, respectively. The blank under Y_0 for $z=6$ means that Eq. (25) has no real roots for that case. It is seen from Table I that, for $z=6$ and $z=8$ and for long wavelength, the contribution of the trilinear terms more than compensates the correction, presented by the factor $(1-2\Delta)$, in Eq. (1). In fact, the result almost coincides with the correction given in Eq. (2), for which the numerical values are listed under K_1. For $z=4$ the term in $(1-2\Delta)$ is not compensated. It is also clear that the fifth-order terms in their approximate form, contribute largely to the final result. Their influence is measured by $K_\Delta-K_0$, which is, for $z=6$ and $z=8$, of the same order of magnitude as K_Δ. For $z=4$ the discrepancy is very large, and one is led to doubt the convergence of the procedure for that 2-dimensional lattice.

For short waves the results in Table II show that Eq. (1), and not Eq. (2) holds with good accuracy. But again, Y_0 for $z=4$ is out of proportion. This fact that $z=6$, $\Delta=0$ gives no solutions is of mathematical, rather than physical interest. The results can be summarized by saying that for 3-dimensional lattices the Holstein-Primakoff representation seems to give a quite rapid convergence for long wavelength, while the other representation converges very rapidly for short wavelength. One can therefore expect a gradual transition from Eq. (2) with $\sigma\rightarrow 2\sigma$ to Eq. (1) when the wavelength decreases from infinite values to the values defined by $\gamma=0$.

Note added in proof. For K_1 in Table I, I took twice the values of reference 3. This makes the correction to the *mean* energy into the correction to the *quasi-particle* energy, as pointed out to me by Dr. F. Keffer.

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