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A simple derivation of the three magnon bound state equation

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Abstract. A simple derivation of the equation for determining the bound states of three magnons in the Heisenberg linear chain with longitudinal anisotropy is given. The present method utilizes nothing more than the Schrödinger equation and Faddeev's three body equations, and avoids the introduction of the ideal spin wave Hilbert space.

Keywords. Three magnon bound state equation; Faddeev's Theory.

1. Introduction

The old problem of spin-wave interactions for the Heisenberg Hamiltonian

$$\mathcal{H} = -\tfrac{1}{2} J \sum_{i,\delta} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+\delta} \tag{1}$$

(**i** denotes the lattice sites; δ joins a site to its nearest neighbours) still retains some interest. Many years ago, Bethe (1931) considered the linear chain, described by the Hamiltonian

$$\mathcal{H} = -J \sum_{i=1}^{N} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} \tag{2}$$

($J > 0$, $N+1 \equiv 1$, i.e. periodic boundary conditions) and showed that the interactions were strong enough to produce bound states of two or more spin waves. In one, two and three dimensions, the interaction of just two spin waves leads to a soluble problem. Its solution was started by Dyson (1956) in his classic work on the Hamiltonian (1) and completed by the work of Hanus (1963) and Wortis (1963). Fukuda and Wortis (1963) gave an extremely simple derivation of the solution. The problem has been studied by several others (Boyd and Callaway 1965, Katsura 1965) from different angles.

Since Bethe's predictions were made, almost forty years elapsed before the bound spin wave states were detected experimentally by Torrance and Tinkham (1969 a, b) in the far-infrared transmission studies on $CoCl_2 \cdot 2H_2O$ at helium temperatures. They found 2, 3, 4 and 5 spin wave bound states. Actually $CoCl_2 \cdot 2H_2O$ has strong longitudinal and transverse anisotropy. Taking advantage of the longitudinal anisotropy, Torrance and Tinkham explained the data by a slight variation of the Ising model. They also pointed out that the transverse anisotropy in $CoCl_2{\cdot}2H_2O$, though weaker than the longitudinal part, facilitated the observation of the bound states. The introduction of the transverse anisotropy complicates the theoretical problem very much, although Baxter (1971 a, b), in a remarkable work, has succeeded in solving the ground state energy problem of the completely anisotropic linear chain

$$\mathcal{H} = -\sum_{i=1}^{N} \left[J_x S_i^x S_{i+1}^x + J_y S_i^y S_{i+1}^y + J_z S_i^z S_{i+1}^z \right] \tag{3}$$

($J_x \neq J_y \neq J_z$). The transverse anisotropy is still sufficiently weak so that it can be left out as a first approximation. The mathematical problem then becomes much more tractable, almost in the same manner as (2) is.

The Hamiltonian with only longitudinal anisotropy we shall write as

$$\mathcal{H} = -J \sum_{i=1}^{N} \left[S_i^z S_{i+1}^z + \sigma \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \right) \right] \tag{4}$$

This has been studied by Kastelijn (1952), Orbach (1958), Walker (1959), Griffiths (1964), Katsura and Inawashiro (1964), des Cloizeaux and Gaudin (1966), Yang and Yang (1966 a, b, c) and Flicker and Leff (1968). In view of the experimental situation, one might pose the problem of computing the various spin wave bound states of (4), for all values of $|\sigma|$ between 0 and 1 (the dominantly ferromagnetic situation). In fact with two spin waves in interaction the complete solution is obtained by Orbach (1958), following the Bethe analysis, and by Wortis (1963). For arbitrary σ their generalized equations have not been solved for three or more spin waves.

The bound state problem for three interacting spin waves for (2) was solved by Majumdar (1970) by a new line of attack. He utilized the rigorous quantum mechanical treatment of the three body problem by Faddeev (1961) (Newton 1966) and derived an integral equation for the bound state eigenvalue. Majumdar and Mukhopadhyay (1970) computed the eigenvalues for arbitrary σ. There are three steps in this calculation. First, the spin Hamiltonian is converted into a Hamiltonian for interacting Bose particles by Dyson's construction. The ferromagnetic ground state becomes the vacuum, the single particle states are the ordinary spin waves. The spins at each site have a kinematical restriction—there are $(2S+1)$ states associated with a spin of magnitude S on a site. The harmonic oscillator introduced at each site in lieu of the spins have no such restriction. Over this extended basis, a new Hamiltonian is constructed such that the physical scattering matrix elements of the original spin problem are correctly reproduced. This new operator is in fact non-hermitian. [A general discussion of possible Dyson-like construction is given by Dembinski (1964)]. In the second stage the two spin wave interaction is solved completely in terms of the t-matrix and it is observed that this t-matrix is separable. The importance of this simplification was first realized in connection with the Faddeev equations by Lovelace (1964). Finally, the Faddeev equations for the 3 spin waves are written down and simplified, thanks to the separability of the two particle t-matrix, into an integral equation for the 3-magnon bound states.

The first step is complicated. The full capability of the Dyson construction is required in discussing thermodynamics of spin waves, but it seems that for the dynamical problem of three bound magnons a simpler method, for example a generalization of the Fukuda and Wortis (1963) method, ought to suffice. This work presents such a generalization.

The method, just as the original method, works in one, two and three dimensions, but the solution for the eigenvalues has so far been possible in one dimension. We shall restrict ourselves to the exposition of the one-dimensional situation for $S=\frac{1}{2}$.

2. The two-magnon problem

We write (4) as

$$\mathcal{H}=\tfrac{1}{2}\sum_{i,j} \mathcal{J}(i,j)[S_i^z S_j^z+\tfrac{1}{2}\sigma(S_i^+ S_j^- + S_i^- S_j^+)] \tag{5}$$

$\mathcal{J}(i,j)$ will be taken to be zero unless i and j are nearest neighbour sites, and $-\mathcal{J}$ if they are. Also $\mathcal{J}(i,j)=\mathcal{J}(j,i)$. As ground state $|0\rangle$, we take the all-spins down state with energy E_0.

$$\begin{aligned}|0\rangle &=\beta(1)\,\beta(2)\ldots\ldots\ldots\beta(\mathcal{N})\\ \mathcal{H}\,|0\rangle &=E_0\,|0\rangle\end{aligned} \tag{6}$$

Let the one spin wave state be

$$\psi=\sum_l U(l) S_l^+\,|0\rangle \tag{7}$$

with energy E_1 or excitation energy $\varepsilon_1=E_1-E_0$. Then from $\mathcal{H}\psi=E_1\psi$ we get

$$\varepsilon_1\psi=\sum_l U(l)\left[\mathcal{H},\, S_l^+\right]|0\rangle \tag{8}$$

Using the standard commutation rules

$$\left[S_j^z,\, S_k^\pm\right]=\pm\, S_j^\pm \delta_{jk},\ \left[S_j^+,\, S_k^-\right]=2\delta_{jk}\, S_j^z \tag{9}$$

we get

$$\left[\mathcal{H},\, S_l^+\right]=\sum_i \mathcal{J}(i,\, l)\,\left[S_l^+ S_i^z - \sigma S_i^+ S_l^z\right] \tag{10}$$

As

$$S_i^z\,|0\rangle=-\tfrac{1}{2}\,|0\rangle,\ \text{for every } i,$$

we have from (8) and (10)

$$\varepsilon_1\,\psi=\tfrac{1}{2}\sum_l U(l)\sum_i \mathcal{J}(i,\, l)\,\left(-S_l^+ + \sigma\, S_i^+\right)|0\rangle$$

or,

$$\begin{aligned}\sum_l\left[\varepsilon_1+\tfrac{1}{2}\sum_i \mathcal{J}(i,\, l)\right]U(l)\, S_l^+\,|0\rangle &=\tfrac{1}{2}\sigma\sum_l\sum_i U(l)\mathcal{J}(i,l) S_i^+\,|0\rangle\\ &=\tfrac{1}{2}\sigma\sum_l\sum_i U(i)\mathcal{J}(i,\, l)\, S_l^+\,|0\rangle\end{aligned} \tag{11}$$

Follows the difference equation for $U(l)$:

$$(\varepsilon_1-\mathcal{J})\,U(l)=-\tfrac{1}{2}\sigma\mathcal{J}(U(l+1)+U(l-1)) \tag{12}$$

The solution is

$$U(l)=N^{-\frac{1}{2}}\exp(ikl)$$
$$k=2\pi\lambda/N,\ \lambda=0,1,\ldots\ldots,N-1 \qquad (13)$$
$$\varepsilon_1=J(1-\sigma\cos k)$$

The two spin wave state can be written as

$$\psi=\sum_{l,m}U(l,m)\,S_l^+S_m^+|0\rangle \qquad (14)$$

As $\left[S_l^+, S_m^+\right]=0$, we must have symmetry between l and m, $U(l,m)=U(m,l)$. Also for $S=\frac{1}{2}$, $S_l^+S_l^+|0\rangle$ is identically zero, so $U(l,l)$ is undefined. The excitation energy ε_2 for this state is given by

$$\varepsilon_2\psi=\sum_{l,m}U(l,m)\sum_i J(i,l)\left(S_l^+S_i^z-\sigma S_i^+S_l^z\right)S_m^+|0\rangle+$$
$$+\sum_{l,m}U(l,m)\sum_i J(i,m)S_l^+\left(S_m^+S_i^z-\sigma S_i^+S_m^z\right)|0\rangle \qquad (15)$$

In pushing the S^z operators to the right we remember that i can be equal to m.

$$\varepsilon_2\psi=\sum_{l,m}U(l,m)\sum_i J(i,l)\left[S_l^+S_m^+S_i^z+S_l^+S_m^+\delta_{im}-\sigma S_i^+S_m^+S_l^z\right.$$
$$\left.-\sigma S_i^+S_m^+\delta_{lm}\right]|0\rangle+\sum_{l,m}U(l,m)\sum_i J(i,m)\left(S_l^+S_m^+S_i^z-\sigma S_l^+S_i^+S_m^z\right)|0\rangle$$

or

$$\sum_{l,m}\left[\varepsilon_2+\tfrac{1}{2}\sum_i J(i,l)+\tfrac{1}{2}\sum_i J(i,m)\right]U(l,m)S_l^+S_m^+|0\rangle$$
$$=\tfrac{1}{2}\sigma\sum_{l,m}\sum_i U(l,m)J(i,l)\,S_i^+S_m^+|0\rangle+\tfrac{1}{2}\sigma\sum_{l,m}\sum_i U(l,m)J(i,m)S_l^+S_i^+|0\rangle-$$
$$-\tfrac{1}{2}\sigma\sum_{l,m}\sum_i U(l,m)J(i,l)\,S_i^+S_m^+\delta_{lm}|0\rangle+$$
$$+\sum_{l,m}U(l,m)J(l,m)S_l^+S_m^+|0\rangle \qquad (16)$$

Now

$$\sum_{l,m}\sum_i U(l,m)J(i,l)\,S_i^+S_m^+|0\rangle=\sum_{l,m}\sum_i U(i,m)J(l,i)\,S_l^+S_m^+|0\rangle,$$
$$\sum_{l,m}\sum_i U(l,m)J(i,m)\,S_l^+S_i^+|0\rangle=\sum_{l,m}\sum_i U(l,i)\,J(m,i)\,S_l^+S_m^+|0\rangle \qquad (17)$$

We treat the delta function part symmetrically:

$$\sum_{l,m,i}U(l,m)\,J(i,l)\,S_i^+S_m^+\delta_{lm}$$
$$=\tfrac{1}{2}\sum_{l,i}U(l,l)J(i,l)S_i^+S_l^++\tfrac{1}{2}\sum_{m,i}U(m,m)J(i,m)S_i^+S_m^+$$
$$=\tfrac{1}{2}\sum_{l,m}(U(l,l)+U(m,m))\,J(l,m)S_l^+S_m^+ \qquad (18)$$

From (16), (17) and (18) we get

$$\sum_{l,m}(\varepsilon_2-2\mathcal{J})U(l,m)\,S_l^+S_m^+\,|\,0\,\rangle=\tfrac{1}{2}\sum_{l,m}\sum_i U(i,m)\mathcal{J}(l,i)S_l^+S_m^+\,|\,0\,\rangle$$

$$+\tfrac{1}{2}\sigma\sum_{l,m}\sum_i U(l,i)\,\mathcal{J}(m,i)\,S_l^+S_m^+\,|\,0\,\rangle$$

$$-\tfrac{1}{2}\sum_{l,m}\mathcal{J}(l,m)[\sigma\{U(l,l)+U(m,m)\}-2U(l,m)]\,S_l^+S_m^+\,|\,0\,\rangle \tag{19}$$

Hence

$$(\varepsilon_2-2\mathcal{J})\,U(l,m)=\tfrac{1}{2}\sigma\sum_i U(i,m)\mathcal{J}(l,i)+\tfrac{1}{2}\sigma\sum_i U(l,i)\,\mathcal{J}(m,i)-$$

$$-\tfrac{1}{2}\mathcal{J}(l,m)\,\{\sigma U(l,l)+\sigma U(m,m)-2U(l,m)\} \tag{20}$$

Note that the physically undefined quantities $U(m, m)$ and $U(l, l)$ cancel out of the right hand side of the equation as they should. The Schrödinger equation (15) thus does not involve these. It is convenient, however, to remove undefined character of $U(l, m)$ at $l=m$ so that Fourier transforms can be freely taken. We assume that (20) holds when $l=m$ on the left; this defines $U(l, l)$ in terms of physically significant quantities. Eq. (20) thus hold for all l and m. Define the Fourier transform

$$U(l,m)=\mathcal{N}^{-1}\sum_{k_1,k_2}U(k_1,k_2)\,\exp\,(ik_1l+ik_2m) \tag{21}$$

with $U(k_1, k_2)=U(k_2, k_1)$ by symmetry of l and m. Eq. (20) gives

$$[\varepsilon_2-2\mathcal{J}+\sigma\mathcal{J}(\cos k_1+\cos k_2)]\;U(k_1,k_2)$$

$$=-\frac{1}{2\mathcal{N}^2}\sum_{l,m}\exp(-ik_1l-ik_2m)\mathcal{J}(l,m)\sum_{k'_1\,k'_2}\{\sigma\exp\,[i\,(k'_1+k'_2)l]+$$

$$+\sigma\exp\,[i(k'_1+k'_2)m]-2\exp\,(ik'_1l+ik'_2m)\}U(k'_1,k'_2) \tag{22}$$

Define the centre of mass and relative momentum

$$p=k_1+k_2,\;\;p'=k'_1+k'_2,\;\;q=\tfrac{1}{2}\,(k_1-k_2),\;\;q'=\tfrac{1}{2}(k'_1-k'_2) \tag{23}$$

Eq. (23) reduces to

$$[\varepsilon_2-2\mathcal{J}+2\sigma\mathcal{J}\cos\tfrac{1}{2}p\cos q]U(p,q)$$

$$=\frac{\mathcal{J}}{\mathcal{N}}\sum_{p',q'}\delta(p-p')\{2\sigma\cos q\cos\tfrac{1}{2}p'-2(\cos q\cos q'+\sin q\sin q')\}U(p',q')$$

$$=\frac{2\mathcal{J}}{\mathcal{N}}\sum_{q'}\cos q(\sigma\cos\tfrac{1}{2}p-\cos q')\;U(p,q') \tag{24}$$

The last line follows as $U(p, -q)=U(p, q)$. The continuum of the two particle states is given by $\varepsilon_2=2\mathcal{J}\,[1-\sigma\cos\frac{1}{2}p\cos q]$, while the bound state is obtained by the solution of the integral equation (24). The bound state condition is

$$1=\frac{2\mathcal{J}}{\pi}\int_0^\pi\frac{\cos q(\sigma\cos\frac{1}{2}p-\cos q)\,dq}{\varepsilon_2-2\mathcal{J}+2\sigma\mathcal{J}\cos\frac{1}{2}p\cos q} \tag{25}$$

and the bound state energy is

$$\varepsilon_{2B}=\mathcal{J}\,(1-\sigma^2\cos^2\tfrac{1}{2}p) \tag{26}$$

We shall not write down the two particle t-matrix here, as it is derived below in the form required.

3. The three magnon problem

The three spin deviation state is written as

$$\psi=\sum_{l,m,n} U(l,m,n)\, S_l^+ S_m^+ S_n^+ |0\rangle \tag{27}$$

Here $U(l, m, n)$ is symmetric under the permutation group S_3 of three objects. The excitation energy ε_3 of the state (27) is given by

$$\varepsilon_3\psi=\sum_{l,m,n} U(l,m,n)\Big[\sum_i \mathcal{J}(i,l)\left(S_l^+ S_i^z-\sigma S_i^+ S_l^z\right) S_m^+ S_n^+ + S_l^+\sum_i \mathcal{J}(i,m)\left(S_m^+ S_i^z-\sigma S_i^+ S_m^z\right) S_n^+ + S_l^+ S_m^+\sum_i \mathcal{J}(i,n)\left(S_n^+ S_i^z-\sigma S_i^+ S_n^z\right)\Big]|0\rangle \tag{28}$$

First we push all the S^z terms to the extreme right to let them operate on the vacuum state, carefully keeping any non-vanishing commutator. Next we use considerations analogous to Eqs. (17) and (18). We thus arrive at the equation

$$\begin{aligned}(\varepsilon_3-3\mathcal{J})U(l,m,n)=&\tfrac{1}{2}\sigma\sum_i[U(i,m,n)\mathcal{J}(i,l)+U(l,i,n)\mathcal{J}(i,m)+\\&+U(l,m,i)\mathcal{J}(i,n)]-\tfrac{1}{2}\mathcal{J}(l,m)[\sigma U(l,l,n)+\sigma U(m,m,n)-2U(l,m,n)]\\&-\tfrac{1}{2}\mathcal{J}(m,n)[\sigma U(l,m,m)+\sigma U(l,n,n)-2U(l,m,n)]\\&-\tfrac{1}{2}\mathcal{J}(n,l)[\sigma U(l,m,l)+\sigma U(n,m,n)-2U(l,m,n)]\end{aligned} \tag{29}$$

The equation thus derived for the condition that no two of the trio l, m, n could be equal is extended to arbitrary l, m, n by defining the unphysical quantities $U(l, l, n)$ etc. by means of (29). We are then ready to take Fourier transforms:

$$U(l,m,n)=\mathcal{N}^{-\frac{3}{2}}\sum_{k_1,k_2,k_3} U(k_1,k_2,k_3)\exp[i(k_1l+k_2m+k_3n)] \tag{30}$$

We obtain

$$\begin{aligned}&[\varepsilon_3-3\mathcal{J}+\sigma\mathcal{J}(\cos k_1+\cos k_2+\cos k_3)]\,U(k_1,k_2,k_3)\\&=-\frac{1}{2\mathcal{N}^{\frac{3}{2}}}\sum_{l,m,n}\exp[-i(k_1l+k_2m+k_3n)]\,[\mathcal{J}(l,m)\{\sigma U(l,l,n)+\\&+\sigma U(m,m,n)-2U(l,m,n)\}+\mathcal{J}(m,n)\{\sigma U(l,m,m)+\sigma U(l,n,n)-\\&-2U(l,m,n)\}+\mathcal{J}(n,l)\{\sigma U(l,m,l)+\sigma U(n,m,n)-2U(l,m,n)\}]\end{aligned} \tag{31}$$

Consider the reduction of the first term on the right hand side. We have

$$\begin{aligned}&\frac{1}{\mathcal{N}^3}\sum_{l,m,n}\exp\{-i(k_1l+k_2m+k_3n)\}\mathcal{J}(l,m)\sum_{k_1',k_2',k_3'}\{\sigma\exp[i(k_1'l+k_2'l+k_3'n)]+\\&+\sigma\exp[i(k_1'm+k_2'm+k_3'n)]-2\exp[i(k_1 l+k_2'm+k_3'n]\}U(k_1',k_2',k_3')\\&=-\frac{2\mathcal{J}}{\mathcal{N}}\sum_{k_1',k_2',k_3'}\delta(k_1+k_2+k_3-k_1'-k_2'-k_3')\,\delta(k_1+k_2-k_1'-k_2')\times\\&\times[\sigma\cos\tfrac{1}{2}\{(k_1-k_2)+(k_1'+k_2')\}+\sigma\cos\tfrac{1}{2}\{(k_1-k_2)-(k_1'+k_2')\}\\&\quad-2\cos\tfrac{1}{2}\{(k_1-k_2)-(k_1'-k_2')\}]\,U(k_1',k_2',k_3')\end{aligned} \tag{32}$$

We now define

$$K=k_1+k_2+k_3, \qquad K'=k'_1+k'_2+k'_3,$$
$$p_3=k_1+k_2, \qquad p'_3=k'_1+k'_2,$$
$$q_3=\tfrac{1}{2}(k_1-k_2), \qquad q=\tfrac{1}{2}(k'_1-k'_2) \tag{33}$$

Eq. (32) takes the compact form

$$-\frac{4J}{N}\sum_{K',p'_3,q'_3}\delta(K-K')\delta(p_3-p'_3)[\sigma\cos q_3\cos\tfrac{1}{2}p'_3-\cos q_3\cos q'_3-\sin q_3\sin q'_3]\times$$
$$\times U(K',p'_3,q'_3)$$
$$=-\frac{4J}{N}\sum_{K',p'_3,q'_3}\delta(K-K')\delta(p_3-p'_3)\cos q_3\,(\sigma\cos\tfrac{1}{2}p'_3-\cos q'_3)U(K',p'_3,q'_3) \tag{34}$$

The last step uses the symmetry $U(K',p'_3,-q'_3)=U(K',p'_3\, q'_3)$.

Clearly, as in (33), we could define two other sets (p_2, q_2) and (p_1, q_1) obtained by cyclic permutation of the indices 1, 2, 3. All these decompositions are equivalent and we have

$$|\,k_1, k_2, k_3\,\rangle \equiv |\,K, p_1, q_1\,\rangle_1 \equiv |\,K, p_2, q_2\,\rangle_2 \equiv |\,K, p_3, q_3\,\rangle_3 \tag{35}$$

the subscripts 1, 2, 3 referring to the particular decomposition. The reduction of the last two terms of (31) can be achieved with the help of these sets (p_1, q_1) and (p_2, q_2), exactly as (p_3, q_3) is used in (34). Eq. (31) finally takes the form

$$[\varepsilon_3-3J+\sigma J(\cos k_1+\cos k_2+\cos k_3)]U([k])=\sum_{[k']}\langle\,[k]\,|\,V\,|\,[k']\,\rangle\,U([k']) \tag{36}$$

where the total interaction can be written as

$$\langle\,[k]|\,V|[k']\,\rangle=\frac{2J}{N}\,\delta(K-K')[\delta(p_3-p'_3)\cos q_3\,(\sigma\cos\tfrac{1}{2}p_3-\cos q'_3)+$$
$$+\delta(p_2-p'_2)\cos q_2(\sigma\cos\tfrac{1}{2}p_2-\cos q'_2)+\delta(p_1-p'_1)\cos q_1\,(\sigma\cos\tfrac{1}{2}p_1-\cos q'_1)] \tag{37}$$

Compare this with Eq. (25). The full interaction is a sum of three two-body interactions, the momentum representation of each is given explicitly in (37). Observing which two of the three spin waves interact, we use a particular decomposition of the set (k_1, k_2, k_3) or (k'_1, k'_2, k'_3). This last fact is implied by enclosing the momenta in square brackets. The overall momentum conservation is given by $\delta(K-K')$: this causes no difficulty. The existence of the other delta functions $\delta(p_3-p'_3)$ etc., indicating one spin wave remains a spectator while the other two interact, causes difficulty in mathematical manipulations. Precisely this is overcome in Faddeev's equations for the three body problem.

Briefly these equations are as follows. Let the three body problem be set as

$$(E-H_0)U=VU\equiv(V_1+V_2+V_3)U \tag{38}$$

where H_0 is the diagonal part in momentum representation. The three particle T-matrix is then written as

$$T=T^1+T^2+T^3 \tag{39}$$

with

$$
\begin{aligned}
T^1 &= T_1 + T_1 G_0 (T^2 + T^3) \\
T^2 &= T_2 + T_2 G_0 (T^3 + T^1) \\
T^3 &= T_3 + T_3 G_0 (T^1 + T^2)
\end{aligned} \tag{40}
$$

and

$$
G_0 = (E - H_0)^{-1} \tag{41}
$$

The operators T_i's are derived from the two body potentials

$$
\begin{aligned}
T_1 &= V_1 + V_1 G_0 T_1 \\
T_2 &= V_2 + V_2 G_0 T_2 \\
T_3 &= V_3 + V_3 G_0 T_3
\end{aligned} \tag{42}
$$

These are really the two-particle t-matrices but because they contain G_0 and operate in three particle Hilbert space, they are actually obtained by off-shell extension of the t-matrix that would be derived from (25). We shall directly solve (42).

Take the equation for T_3, for example. From (34) we identify V_3 and use the set (K, p_3, q_3), subscript 3,

$$
\begin{aligned}
{}_3\langle [k] \mid T_3 \mid [k'] \rangle_3 = {} & \frac{2J}{N} \delta(K-K')\delta(p_3-p_3') \cos q_3 \, (\sigma \cos \tfrac{1}{2}p_3 - \cos q_3') + \\
& + \frac{2J}{N} \sum_{[k'']} \frac{\delta(K-K'')\delta(p_3-p_3'') \cos q_3 (\sigma \cos \tfrac{1}{2}p_3 - \cos q_3'')}{\varepsilon_3 - 3J + 2\sigma J \cos \tfrac{1}{2}p_3'' \cos q_3'' + \sigma J \cos (K - p_3'')} \, {}_3\langle [k''] | T_3 | [k'] \rangle_3
\end{aligned} \tag{43}
$$

Putting

$$
{}_3\langle [k] \mid T_3 \mid [k'] \rangle_3 = \frac{2J}{N} \delta(K-K')\delta(p_3-p_3') \cos q_3 \phi\, (q_3') \tag{44}
$$

we get

$$
\phi(q_3') = (\sigma \cos \tfrac{1}{2}p_3 - \cos q_3') + \frac{2J}{N} \sum_{q_3''} \frac{\cos q_3'' (\sigma \cos \tfrac{1}{2}p_3 - \cos q_3'') \phi(q_3')}{\varepsilon_3 - 3J + \sigma J \cos (K - p_3) + 2\sigma J \cos \tfrac{1}{2}p_3 \cos q_3''}
$$

or

$$
\phi(q_3') = (\sigma \cos \tfrac{1}{2}p_3 - \cos q_3') / D(\varepsilon_3, K, p_3\, \sigma) \tag{45}
$$

where

$$
\begin{aligned}
D(\varepsilon_3, K, p_3, \sigma) &= 1 - \frac{2J}{N} \sum_q \frac{\cos q \, (\sigma \cos \tfrac{1}{2}p_3 - \cos q)}{\varepsilon_3 - 3J + \sigma J \cos (K - p_3) + 2\sigma J \cos \tfrac{1}{2}p_3 \cos q} \\
&= [\tfrac{3}{2} - \omega - \tfrac{1}{2}\sigma \cos (K-p_3) - \{\tfrac{3}{2} - \omega - \tfrac{1}{2}\sigma \cos (K-p_3) - \sigma^2 \cos^2 \tfrac{1}{2} p_3\} \times \\
&\quad \times \left(1 - \frac{\sigma^2 \cos^2 \tfrac{1}{2}p_3}{[\tfrac{3}{2} - \omega - \tfrac{1}{2}\sigma \cos (K-p_3)]^2}\right)^{-\frac{1}{2}} \Bigg] \Big/ \sigma^2 \cos^2 \tfrac{1}{2}p_3
\end{aligned} \tag{46}
$$

with $\omega = \varepsilon_3 / 2J$.

So*

*One might be puzzled by the difference of a factor 2 between this equation and Eq. (76) of Majumdar (1970). This arises as the latter explicitly uses the creation and annihilation operators for bosons and takes exchange automatically into account. The present work leaves out exchange explicitly; it is, of course, known that exchange is equal to the direct term for these bosons.

$$ {}_3\langle [k]|T_3|[k']\rangle_3=\frac{2J}{N}\,\delta(K-K')\delta(p_3-p_3')\cos q_3(\sigma\cos\tfrac{1}{2}p_3-\cos q_3')/D(\varepsilon_3\, K, p_3, \sigma) \tag{47}$$

Expressions for T_1 and T_2 can be similarly written down in their respective sets subscripted by 1 and 2.

Consider now the first of Eq. (40). For T^i we are to use set i. Thus

$$ {}_1\langle K, p_1, q_1, | T^1|[k']\rangle ={}_1\langle K, p_1, q_1| T_1| [k']\rangle + \sum_{[k'']}\langle K, p_1, q_1| T_1| [k'']\rangle\times $$
$$ \times\frac{\{\langle [k'']| T^2| [k']\rangle+\langle [k'']| T^3| [k']\rangle\}}{\varepsilon_3-3J+\sigma J(\cos k_1''+\cos k_2''+\cos k_3'')} \tag{48}$$

For T^2, we must have $\langle [k'']| ={}_2\langle K'', p_2'', q_2''|$ and for T^3, we must have $\langle [k'']| ={}_3\langle K'', p_3'', q_3''|$. On the other hand, for T_1 we must express $|[k'']\rangle$ in terms of the set 1. Let

$$ \begin{aligned} |[k'']\rangle &\equiv |K'', p_2'', q_2''\rangle_2\equiv |K'', \bar{p}_2'', \bar{q}_2''\rangle_1 \\ |[k'']\rangle &\equiv |K'', p_3'', q_3''\rangle_3\equiv |K'', \bar{p}_3'', \bar{q}_3''\rangle_1 \end{aligned} \tag{49}$$

We use (33) to work out the transformation (49):

$$ \begin{aligned} \bar{p}_2'' &=K''-\tfrac{1}{2}p_2''+q_2'', & \bar{q}_2'' &=\tfrac{1}{2}(K''-\tfrac{3}{2}p_2''-q_2'') \\ \bar{p}_3'' &=K''-\tfrac{1}{2}p_3''-q_3'', & \bar{q}_3'' &=\tfrac{1}{2}(-K''+\tfrac{3}{2}p_3''-q_3'') \end{aligned} \tag{50}$$

We then have

$$ \begin{aligned} &{}_1\langle K, p_1, q_1 | T_1| [k'']\rangle_2={}_1\langle K, p_1, q_1 | T_1| K'', \bar{p}_2'', \bar{q}_2''\rangle_1 \\ &=\frac{2J}{N}\,\delta(K-K'')\delta(p_1-\bar{p}_2'')\cos q_1\,(\sigma\cos\tfrac{1}{2}p_1-\cos\bar{q}_2'')/D(\varepsilon_3, K_1, p_1, \sigma) \\ &=\frac{2J}{N}\,\delta(K-K'')\,\delta(p_1-K+\tfrac{1}{2}p_2''-q_2'')\times \\ &\quad\times\cos q_1\,[\sigma\cos\tfrac{1}{2}p_1-\cos\tfrac{1}{2}(K''-\tfrac{3}{2}p_2''-q_2'')]/D(\varepsilon_3, K, p_1, \sigma) \end{aligned} \tag{51}$$

Eq. (48) becomes

$$ \begin{aligned} &{}_1\langle K, p_1, q_1 | T^1| [k']\rangle ={}_1\langle K, p_1, q_1 | T_1| [k']\rangle_1+ \\ &+\frac{2J}{N}\,\frac{\cos q_1}{D(\varepsilon_3, K, p_1, \sigma)}\times \\ &\times\sum_{K'', p_2'', q_2''}\frac{\delta(K-K'')\delta(p_1-K''+\tfrac{1}{2}p_2''-q_2'')\,[\sigma\cos\tfrac{1}{2}p_1-\cos\tfrac{1}{2}(-\tfrac{3}{2}p_2''+K''-q_2'')]}{\varepsilon_3-3J+2\sigma J\cos\tfrac{1}{2}p_2''\cos q_2''+\sigma J\cos(K-p_2'')}\times \\ &\qquad\times{}_3\langle K'', p_2'', q_2'' | T^2| [k']\rangle+ \\ &+\frac{2J}{N}\,\frac{\cos q_1}{D(\varepsilon_3, K, p_1, \sigma)}\times \end{aligned} $$

$$\times \sum_{K'', p_3'', q_3''} \frac{\delta(K-K'')\delta(p_1-K''+\tfrac{1}{2}p_3''+q_3'')\,[\sigma\cos\tfrac{1}{2}p_1-\cos\tfrac{1}{2}(\tfrac{8}{2}p_3''-K''-q_3'')]}{\varepsilon_2-3J+2\sigma J\cos\tfrac{1}{2}p_3''\cos q_3''+\sigma J\cos(K-p_3'')} \times$$

$$\times\, {}_3\langle K'', p_3'', q_3'' \,|\, T^3 \,|\, [k'] \rangle \qquad (52)$$

We now put, using (51),

$${}_1\langle K, p_1, q_1, | T^1 | [k'] \rangle = \delta(K-K')\cos q_1\, \Psi_1, \text{ etc.}$$
$${}_1\langle K, p_1, q_1, | T_1 | [k'] \rangle_1 = \delta(K-K')\cos q_1, \chi_1, \text{ etc.} \qquad (53)$$

Thus

$$\Psi(p_1) = \chi_1 + \frac{2J}{N}\frac{1}{D(\varepsilon_3, K, p_1, \sigma)} \times$$
$$\times \sum_{p''} \frac{[\sigma\cos\tfrac{1}{2}p_1-\cos(K-\tfrac{1}{2}p_1-p_2'')]\cos(K-p_1-\tfrac{1}{2}p_2'')\,\Psi_2(p_2'')}{\varepsilon_3-3J+\sigma J\cos(K-p_2'')+2\sigma J\cos\tfrac{1}{2}p_2''\cos(K-p_1-\tfrac{1}{2}p_2'')} +$$
$$+\frac{2J}{N}\cdot\frac{1}{D(\varepsilon_3, K, p_1, \sigma)}\sum_{p_3''}\frac{[\sigma\cos\tfrac{1}{2}p_1-\cos(K-\tfrac{1}{2}p_1-p_3'')]\cos(K-p_1-\tfrac{1}{2}p_3'')\Psi_3(p_3'')}{\varepsilon_3-3J+\sigma J\cos(K-p_3'')+2\sigma J\cos\tfrac{1}{2}p_3''\cos(K-p_1-\tfrac{1}{2}p_3'')} \qquad (54)$$

The homogeneous equation leads to the bound state equation

$$\Psi(p_1) = \frac{4J}{N}\sum_{p_2}\frac{[\sigma\cos\tfrac{1}{2}p_1-\cos(K-\tfrac{1}{2}p_1-p_2)]\cos(K-p_1-\tfrac{1}{2}p_2)\,\Psi(p_2)}{D(\varepsilon_3, K, p_1, \sigma)\,[\varepsilon_3-3J+\sigma J\cos(K-p_2)+2\sigma J\cos\tfrac{1}{2}p_2\cos(K-p_1-\tfrac{1}{2}p_2)]} \qquad (55)$$

where we utilized the fact that $\Psi_2(p_2)$ is the same function of p_2 as $\Psi_1(p_1)$ is of p_1.

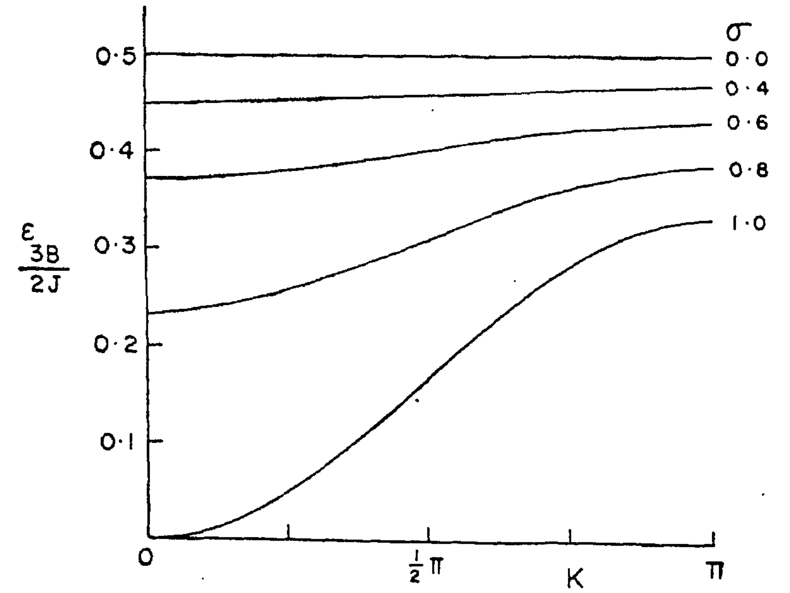

Figure 1. The three magnon bound state energies plotted against the centre of mass momentum for various anisotropies. For $\sigma=0{\cdot}2$, the values are very close to the Ising values $\sigma=0{\cdot}0$. The numbers are actually given in Majumdar and Mukhopadhyay (1970).

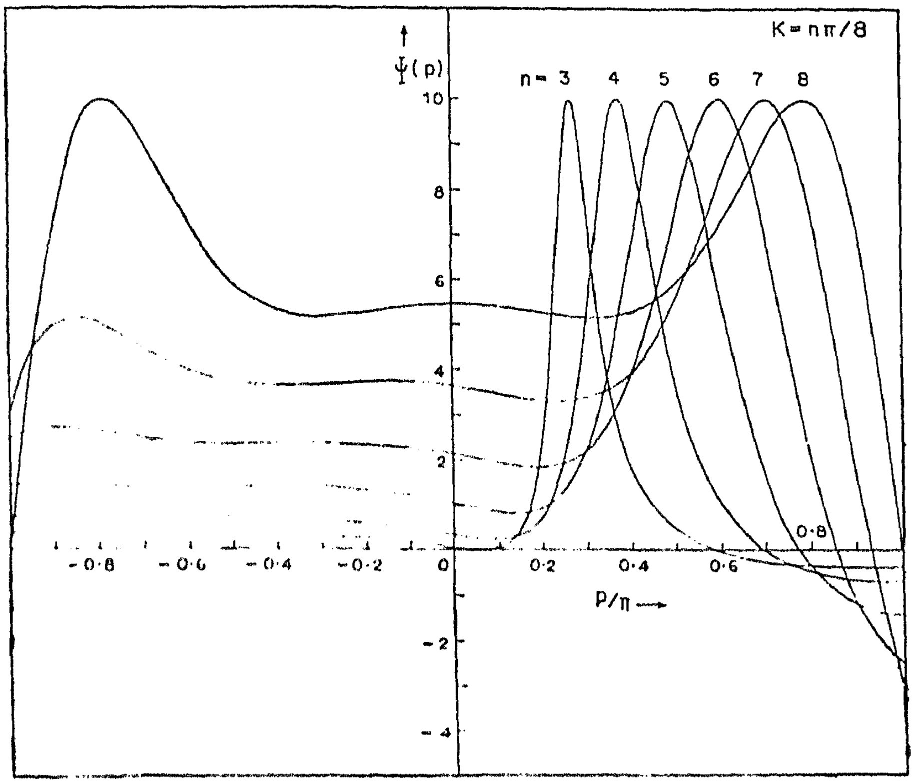

Figure 2. The function $\Psi(p)$ for $\alpha = 1$, and $K = n\pi/8$, $n = 8, 7, 6, 5, 4$, and 3. (Reported in Nuclear Physics and Solid State Physics Symposium BARC, Bombay: Solid State Physics vol. 3, 481 (1972).)

4. Discussion

The equation (55) and its solutions ϵ_{3B} for various values of α were reported earlier (Majumdar and Mukhopadhyay 1976). The solutions were obtained numerically (figure 1). Although it seems feasible, we have not succeeded in getting the functional form $\Psi(p)$ analytically. At $\alpha = 1$, the isotropic case, the energy is known analytically

$$\epsilon_{3B} = \tfrac{1}{3}J(1 - \cos K) \tag{56}$$

The corresponding $\Psi(p)$'s for $K = n\pi/8$, $n = 3, 4, \ldots 8$ are shown in figure 2.

In $CoCl_2{\cdot}2H_2O$ the exchange constants of (3) are in the ratio (Torrance and Tinkham 1969b)

$$J_z : J_x : J_y = 7{\cdot}3 : 2{\cdot}1 : 1{\cdot}0$$

The longitudinal and transverse exchange constants are

$$J_{\parallel} = \tfrac{1}{2}(J_x + J_y) \propto 1{\cdot}55, \qquad J_{\perp} = \tfrac{1}{2}(J_x - J_y) \propto 0{\cdot}55$$

Neglecting transverse anisotropy, we get

$$\alpha = J_{\parallel}/J_z = 0{\cdot}21 \tag{57}$$

Figure 1 shows that the three body bound state energy has negligible bandwidth when plotted against K for such strong longitudinal anisotropy. In the experiment the linewidth is thus extremely small, and one can obtain essentially equivalent answers, as Torrance and Tinkham did, by considering the Ising model.

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