

# Chapter 7

## Spin-Wave Theory

**Abstract** All of the techniques described in the previous chapters are exact methods which work only for particular, but important, special cases. In this chapter we describe a much more general method, due originally to Anderson, which is widely used to obtain results for many different systems. It is referred to as ‘spin-wave theory’ as it gives results for the energies of the elementary excitations or spin waves. The method works for both ferromagnets and antiferromagnets, it works in 2D and 3D as well as 1D, and it works for arbitrary spin – not just for spin-1/2. The ferromagnetic version is rather simple and the results are usually exact. The antiferromagnetic version is more complicated and the results are approximate. However, these results are still in reasonable correspondence with exact results, where these are known, and the best of other approximate methods.

### 7.1 Introduction

The special mathematical techniques introduced for  $S = \frac{1}{2}$  chains, namely the Bethe Ansatz for Heisenberg coupling and the Jordan-Wigner transformation for the  $XY$ -model, do not work for higher  $S$  or higher dimensions. Spin-wave theory is a much more general method of studying spin-models introduced by Anderson (1952) [1] for ferromagnets and later applied by Oguchi (1963) [2] to antiferromagnets.

Spin-wave (SW) theory is not (in general) exact. However, it has many useful features, some of which are

- a. It is rather simple.
- b. It works for many Hamiltonians and in any number of dimensions.
- c. It gives approximate results for non-zero temperature.
- d. It works for arbitrary  $S$ .
- e. It gives a good physical picture of the excitations.

The basic idea of spin-wave theory is to replace the spin operators by bosons. As we have seen, spin operators behave like fermions on a given site, but like bosons where different sites are concerned. Hence we need to find a way of handling the spin operators on a given site in terms of bosons.

Recall that for  $S = \frac{1}{2}$  and a single site

$$\begin{aligned} S^+|-\rangle &= |+\rangle & S^+|+\rangle &= 0 \\ S^-|-\rangle &= 0 & S^-|+\rangle &= |-\rangle \\ S^z|-\rangle &= -\frac{1}{2}|-\rangle & S^z|+\rangle &= \frac{1}{2}|+\rangle \end{aligned}$$

and all other spin operators can be written in terms of these.

For a general spin  $S$  and a single site the corresponding basis is again the eigenstates of  $S^z$  written as  $|m\rangle$  where the  $2S + 1$  values of  $m$  are

$$m = -S, -S + 1, \dots, S$$

and the states  $|m\rangle$  are orthogonal and normalised (i.e. orthonormal). We refer to  $S - m$  as the number of deviations from the state  $|S\rangle$ , the state of maximum  $S^z$ .

The corresponding operators and eigenvalues are

$$S^+|m\rangle = \sqrt{(S - m)(S + m + 1)}|m + 1\rangle \quad (7.1)$$

$$S^-|m\rangle = \sqrt{(S - m + 1)(S + m)}|m - 1\rangle \quad (7.2)$$

$$S^z|m\rangle = m|m\rangle. \quad (7.3)$$

Special cases for  $m = \pm S$  are  $S^+|S\rangle = 0$  and  $S^-| - S\rangle = 0$ .

We now introduce *boson* operators for a single site which reproduce most of the above properties. There are various ways of doing this but we shall only consider the most useful and widely used, called the *Holstein-Primakoff* transformation.

Let  $a^+$ ,  $a$  be boson creation and destruction operators. We now interpret the number of bosons as the number of deviations from the state  $|S\rangle$ . State  $|m\rangle$  has  $(S - m)$  deviations and the number operator for bosons is  $\hat{n} \equiv a^+a$  so

$$\hat{n}|m\rangle = a^+a|m\rangle = (S - m)|m\rangle. \quad (7.4)$$

Clearly we can represent the operator  $S^z$  as

$$S^z = S - \hat{n} \quad (7.5)$$

since  $S^z|m\rangle = (S - \hat{n})|m\rangle = [S - (S - m)]|m\rangle = m|m\rangle$ . Note that (7.3) is now satisfied.

We now have to represent the  $S^+$  and  $S^-$  operators in terms of the bosons. This is done as follows:

$$S^+ = (2S)^{\frac{1}{2}} \sqrt{1 - \frac{\hat{n}}{2S}} a \quad (7.6)$$

$$S^- = a^+ (2S)^{\frac{1}{2}} \sqrt{1 - \frac{\hat{n}}{2S}} \quad (7.7)$$

*Proof* Clearly  $a|m\rangle$  is a state with one less deviation, i.e.

$$a|m\rangle = A_m|m+1\rangle$$

(recall that less deviations mean higher  $S^Z$ ).

The Hermitian conjugate of this is

$$\langle m|a^+ = A_m^*\langle m+1|$$

and the inner product of these gives

$$\langle m|a^+a|m\rangle = |A_m|^2\langle m+1|m+1\rangle$$

and therefore  $(S-m)\langle m|m\rangle = |A_m|^2\langle m+1|m+1\rangle$ .

Since the states  $|m\rangle$  are orthonormal,  $\langle m|m\rangle = \langle m+1|m+1\rangle = 1$ , and so, choosing  $A_m$  to be real,  $A_m = \sqrt{S-m}$ .

Similarly

$$a^+|m\rangle = B_m|m-1\rangle$$

with  $B_m = \sqrt{S-m}$ .

We can now show that choices (7.6) and (7.7) satisfy (7.1) and (7.2). Using (7.6)

$$\begin{aligned} S^+|m\rangle &= (2S)^{\frac{1}{2}}\sqrt{1 - \frac{\hat{n}}{2S}}a|m\rangle \\ &= (2S)^{\frac{1}{2}}\sqrt{S-m}\sqrt{1 - \frac{\hat{n}}{2S}}|m+1\rangle \\ &= (2S)^{\frac{1}{2}}\sqrt{S-m}\sqrt{1 - \frac{(S-m-1)}{2S}}|m+1\rangle \\ &= \sqrt{S-m}\sqrt{2S-S+m+1}|m+1\rangle \\ &= \sqrt{(S-m)(S+m+1)}|m+1\rangle \end{aligned}$$

which agrees with (7.1). By a similar argument (7.2) is satisfied by (7.7).

Note that the Holstein-Primakoff transformation [(7.5), (7.6), and (7.7)] is exact as far as the states  $|S\rangle, |S-1\rangle, \dots, |0\rangle$  are concerned. However, in principle it is possible to have more than  $S$  bosons, i.e. a state of the form

$$|\psi\rangle = (a^+)^k|S\rangle \quad \text{where } k > m.$$

These states are unphysical and they can never be reached if we use the exact transformation. However, we shall now approximate the transformation and this allows coupling to the unphysical states. The approximation will only be valid provided the admixture of the unphysical states is 'small' in some sense.

Mathematically it is very difficult to handle a transformation involving square roots. The approximation we shall use is based on the assumption that the states of

interest all have small probabilities of having deviations on any particular site and a negligible probability of having two or more deviations on the same site. This is equivalent to saying

- a. The total number of deviations  $N_D$  is  $\ll N$ , i.e.  $\langle \hat{n} \rangle \ll 1$ .
- b. Bound states in which deviations cluster together cannot be treated accurately.

With this assumption we approximate the square root as either

$$\sqrt{1 - \frac{\hat{n}}{2S}} \approx 1 \text{ 'simple SW theory'}$$

or

$$\sqrt{1 - \frac{\hat{n}}{2S}} \approx 1 - \frac{\hat{n}}{4S} \text{ 'interacting SW theory'}$$

Interacting spin-wave theory (which is not covered in this book) can deal with small perturbations to spin-waves obtained using simple spin-wave theory, but it cannot deal with bound states.

For simple SW theory we now obtain a very simple result

$$\begin{aligned} S^+ &\approx (2S)^{\frac{1}{2}} a \\ S^- &\approx (2S)^{\frac{1}{2}} a^+ \\ S^z &= S - a^+ a \end{aligned} \tag{7.8}$$

with the usual boson commutation relation  $[a, a^+] = 1$ . Note that (7.8) refers to a single site. For different sites all operators commute so that

$$\begin{aligned} [a_i, a_j] &= [a_i^+, a_j^+] = 0 \\ [a_i, a_j^+] &= \delta_{ij} \end{aligned}$$

## 7.2 Ferromagnetic Spin-Wave Theory

Consider first the Heisenberg model with nearest neighbour ferromagnetic coupling

$$\mathcal{H} = \frac{J}{2} \sum_j \sum_{\rho} \mathbf{S}_j \cdot \mathbf{S}_{j+\rho}$$

where  $J < 0$ ,  $j$  runs over all sites,  $\rho$  runs over all  $\nu$  neighbours. The ground state (both classical and quantum mechanical) will be a state with all atoms aligned. Usually we take this to be the state in which all atoms are in the  $|+S\rangle$  state. (Other degenerate ground states can be easily constructed from this state by using the lowering operator for the whole system  $\sum_i S_i^-$ ). Writing

$$\mathbf{S}_j \cdot \mathbf{S}_{j+\rho} = S_j^Z S_{j+\rho}^Z + \frac{1}{2}(S_j^+ S_{j+\rho}^- + S_j^- S_{j+\rho}^+)$$

and using (7.8) we get

$$\begin{aligned} \mathcal{H} &\approx \frac{JN\nu}{2} S^2 - \frac{JS}{2} \sum_j \sum_\rho (a_j^+ a_j + a_{j+\rho}^+ a_{j+\rho}) \\ &\quad + \frac{JS}{2} \sum_j \sum_\rho (a_j^+ a_{j+\rho} + a_{j+\rho}^+ a_j) \\ &\quad + \frac{J}{2} \sum_j \sum_\rho a_j^+ a_j a_{j+\rho}^+ a_{j+\rho}. \end{aligned}$$

The last term here involves four boson operators. For consistency with our previous approximation we must neglect this term.

The first term is the energy of the ground state (all  $N$  spins up)  $|SSSS\dots S\rangle$ .

Put  $E_F = \frac{JN\nu S^2}{2}$  (recall that for the ferromagnet  $J$  is negative here), so that

$$\mathcal{H} \approx E_F - \frac{JS}{2} \sum_j \sum_\rho [a_j^+ a_j + a_{j+\rho}^+ a_{j+\rho} - a_j^+ a_{j+\rho} - a_{j+\rho}^+ a_j].$$

This quadratic (or bilinear) Hamiltonian is very easy to diagonalise using a Fourier transform. Define new boson operators

$$\begin{aligned} \alpha_k &= \frac{1}{\sqrt{N}} \sum_j e^{ikj} a_j \\ \alpha_k^+ &= \frac{1}{\sqrt{N}} \sum_j e^{-ikj} a_j^+ \\ a_j &= \frac{1}{\sqrt{N}} \sum_k e^{-ikj} \alpha_k \\ a_j^+ &= \frac{1}{\sqrt{N}} \sum_k e^{ikj} \alpha_k^+ \end{aligned}$$

with  $[\alpha_{k_1}, \alpha_{k_2}^+] = \delta_{k_1 k_2}$ .

In 3D  $k$  is a vector. For example for the simple cubic lattice,

$$k = (\lambda_x, \lambda_y, \lambda_z) \frac{2\pi}{n},$$

with  $\lambda_{x,y,z} = 0, 1, 2, \dots, n-1$ , where  $n = N^{\frac{1}{3}}$ . (Assuming that the number of atoms in each direction  $n$  is the same for each of the three perpendicular directions)

Using this

$$\begin{aligned}\mathcal{H} &= E_F - \frac{JS}{2} \sum_k \sum_\rho (1 + 1 - e^{-ik\rho} - e^{ik\rho}) \alpha_k^+ \alpha_k \\ &= E_F + \sum_k \varepsilon_k \alpha_k^+ \alpha_k\end{aligned}$$

where

$$\varepsilon_k = -JS \sum_\rho (1 - \cos k\rho)$$

These are the energies, relative to the fully aligned ground state, of the ferromagnetic spin-waves.

In 1D  $k$  is a scalar given by  $k = \lambda \frac{2\pi}{N}$ , with  $\lambda = 0, 1, 2, \dots, N-1$ . The energy is

$$\begin{aligned}\varepsilon_k &= -JS[2 - \cos k - \cos(-k)] \\ &= -2JS(1 - \cos k)\end{aligned}$$

so for  $S = \frac{1}{2}$

$$\varepsilon_k = -J(1 - \cos k)$$

which are precisely the energies obtained earlier for the 1-deviation states. The difference now is that we can excite any number of bosons and they will always have energy  $\varepsilon_k$ . Previously, when 2-deviation states were treated exactly we found both ‘free’ spin-waves and bound states. In this approximation the corrections to the ‘free’ state are omitted, and the bound states are not obtained at all.

### 7.3 Antiferromagnetic Spin-Wave Theory

The SW approximation is in some ways more interesting when applied to antiferromagnets. Classically these tend to align with neighbouring atoms antiparallel. We shall consider only bipartite lattices which can be divided into two sublattices, such that all the nearest neighbours of any atom lie on the opposite sublattice, e.g. chain, square, honeycomb, simple cubic, b.c.c., etc. (Non-bipartite lattices are normally frustrated, and the study of such lattices is much more complex and not considered here.) For these lattices the classical ground state has all atoms on one sublattice (sublattice  $A$ ) pointing up (say) and all on sublattice  $B$  down.

We can construct a similar state in quantum mechanics, called the Néel state, in which atoms on sublattice  $A$  are ‘up’, i.e. in the  $|+S\rangle$  state, and those on sublattice  $B$  are ‘down’, i.e. in the  $|-S\rangle$  state. This state however is *not* an eigenstate and so is clearly not the true ground state. Nevertheless we can use it as an approximate

ground state, then use SW theory to find the elementary excitations. Finally we can use these to go back and find suitable corrections to the Néel state.

If the total number of deviations from the Néel state is ‘small’, i.e. if the average value of  $S^z$  does not differ greatly from  $+S$  or  $-S$  for sites on each sublattice respectively, then for sublattice  $A$  we can use same transformation as before

$$S^+ \approx (2S)^{\frac{1}{2}}a; \quad S^- \approx (2S)^{\frac{1}{2}}a^+; \quad S^z = S - a^+a$$

(recall that  $\langle a^+a \rangle \equiv \langle \hat{n} \rangle$ , is ‘small’).

For sublattice  $B$  however, we must use deviations from the  $| - S \rangle$  state. The number of deviations is  $(S + m)$ , e.g. if  $S = 6$  and  $m = -2$  then the number of deviations from  $-S$  is 4, i.e.  $S + m$ . Clearly in this case more deviations correspond to *higher*  $S^z$ . The boson creation operators must therefore lead to states of higher  $m$ . We use the notation  $b^+$  and  $b$  for the creation and destruction operators on the  $B$  sublattice.

Since the operator for the number of deviations is  $b^+b$  we must have

$$b^+b = S + S^z$$

so

$$S^z = -S + b^+b \tag{7.9}$$

Likewise a deviation, created by  $b^+$ , will now correspond to increasing  $S^z$  by one. Hence

$$S^+ \approx (2S)^{\frac{1}{2}}b^+; \tag{7.10}$$

and

$$S^- \approx (2S)^{\frac{1}{2}}b. \tag{7.11}$$

Equations (7.9), (7.10), and (7.11) for the  $B$  sublattice correspond to (7.8) for the  $A$  sublattice.

Let us use subscript  $j$  for the ‘up’ sublattice  $A$  and  $\ell$  for the ‘down’ sublattice  $B$ . ( $j + \rho$  is a nearest neighbour of  $j$  and so will be on the ‘down’ sublattice). We can regard the lattice as consisting of  $N_u$  ‘unit cells’, each of which contains 2 atoms, and a sum over one sublattice is equivalent to a sum over the unit cells. Clearly  $N_u = N/2$ .

The Hamiltonian now becomes

$$\mathcal{H} \approx E_N + \frac{JS}{2} \left( 2 \sum_j \sum_\rho \right) \left[ a_j^+ a_j + b_{j+\rho}^+ b_{j+\rho}^+ + a_j^+ b_{j+\rho}^+ + a_j b_{j+\rho} \right] \tag{7.12}$$

where  $E_N = -\frac{JNS^2\nu}{2}$  ( $J$  is positive now) is the energy of the Néel state (i.e. the expectation value of  $\mathcal{H}$  in the Néel state). The extra factor of 2 is needed since the sum over  $j$  is a sum over one sublattice only. Again we have neglected products of four operators.

Now Fourier transform, introducing

$$c_k = \frac{1}{\sqrt{N_u}} \sum_j e^{ikj} a_j \quad \text{etc.}$$

(similar to the  $\alpha_k$  in the ferromagnetic case) and also

$$d_k = \frac{1}{\sqrt{N_u}} \sum_\ell e^{-ik\ell} b_\ell \quad \text{etc.}$$

The allowed values of  $k$  in 1D are now

$$k = \lambda \frac{2\pi}{N_u} \quad \text{with} \quad \lambda = 0, 1, \dots, N_u - 1 = 0, 1, \dots, \frac{N}{2} - 1.$$

If the lattice spacing in 1D is  $d$ , then the actual wavevector  $q$  of the original lattice is in units of  $1/d$ , i.e.  $q = k/d$ . Because the unit cell of the sublattice is now  $2d$  the wavevectors in this spin-wave approximation are in units of  $1/(2d)$ , i.e.  $q = k/(2d)$ . This means that for the largest value of  $k$ , which is  $2\pi$ , the largest value of  $q$  is  $\pi/d$ . In effect the Brillouin zone is now half the size of the original.

In 2D and 3D the effect is similar but complicated by the fact that the symmetry of the sublattice is in general different to that of the atomic lattice. For example a simple cubic lattice has two f.c.c. sublattices so the Brillouin zone of the sublattice is not related in such a simple way to that of the original lattice.

After Fourier transforming the result is

$$\mathcal{H} = E_N + JS \sum_k \sum_\rho \left[ c_k^+ c_k + d_k^+ d_k + e^{ik\rho} c_k^+ d_k^+ + e^{-ik\rho} c_k d_k \right].$$

We define  $\gamma_k = \frac{1}{\nu} \sum_\rho e^{ik\rho}$  ( $= \cos k$  in 1D). Therefore

$$\mathcal{H} = E_N + JS\nu \sum_k \left[ c_k^+ c_k + d_k^+ d_k + \gamma_k (c_k^+ d_k^+ + c_k d_k) \right] \quad (7.13)$$

This form is reminiscent of the  $\mathcal{H}$  we obtained in XY model. Note however that these are bosons not fermions. Also clearly  $k$  is a ‘constant of the motion’ here: there is no coupling of different  $k$ ’s or coupling of  $k$  and  $-k$ , unlike in the XY-model.

The eigenvectors will involve linear combinations of  $c_k$  and  $d_k^+$ . As we noted in the chapter on the XY-model this was first done by Holstein and Primakoff but it is usually known as a Bogoliubov transformation.



Introduce two new Bose operators  $\alpha_k$  and  $\beta_k$ :

$$\begin{aligned}\alpha_k &= u_k c_k + v_k d_k^+ \\ \beta_k &= u_k d_k + v_k c_k^+\end{aligned}$$

where  $u_k$  and  $v_k$  are constants which can be taken to be real without loss of generality, so that

$$\begin{aligned}\alpha_k^+ &= u_k c_k^+ + v_k d_k \\ \beta_k^+ &= u_k d_k^+ + v_k c_k\end{aligned}$$

From now on the subscript  $k$  will be omitted. Note that both  $c$  and  $d^+$  increase the  $z$ -component of angular motion by one unit and thus so does  $\alpha$  whereas  $c^+$  and  $d$  decrease it by one unit and thus so does  $\beta$ .

These operators are required to have the usual Bose commutation relations, namely

$$[\alpha, \alpha^+] = [\beta, \beta^+] = 1$$

with all other pairs of operators from the set  $\{\alpha, \alpha^+, \beta, \beta^+\}$  commuting.

We can easily show, using the Bose properties of  $c$  and  $d$ , that all these commutation relations are satisfied provided that

$$u^2 - v^2 = 1 \tag{7.14}$$

e.g.

$$\begin{aligned}[\alpha, \alpha^+] &= (uc + vd^+)(uc^+ + vd) - (uc^+ + vd)(uc + vd^+) \\ &= u^2[c, c^+] - v^2[d, d^+] = u^2 - v^2 = 1\end{aligned}$$

and

$$\begin{aligned}[\alpha, \beta] &= (uc + vd^+)(ud + vc^+) - (ud + vc^+)(uc + vd^+) \\ &= u^2(cd - dc) + v^2(d^+c^+ - c^+d^+) + uv(d^+d + cc^+ - dd^+ - cc^+) \\ &= 0 + 0 + uv([c, c^+] - [d, d^+]) = uv(1 - 1) = 0\end{aligned}$$

Now consider the operator which gives the total number of excitations of the two types

$$\begin{aligned}\alpha^+\alpha + \beta^+\beta &= (uc^+ + vd)(uc + vd^+) + (ud^+ + vc)(ud + vc^+) \\ &= (u^2 + v^2)(c^+c + d^+d) + 2uv(c^+d^+ + cd) + 2v^2.\end{aligned}$$

We choose the ratio of coefficients to match the ratio in Eq. (7.13), namely

$$\frac{2uv}{u^2 + v^2} = \gamma \quad (7.15)$$

From Eqs.(7.14) and (7.15) it follows that

$$\frac{u}{v} = \frac{1 \pm s}{\gamma} \quad (7.16)$$

where  $s = +\sqrt{1 - \gamma^2}$ . Clearly  $s^2 = 1 - \gamma^2$  and  $\gamma^2 = 1 - s^2$ .

If  $\frac{u}{v} = \frac{1+s}{\gamma}$  and  $u^2 - v^2 = 1$  then

$$\begin{aligned} v^2 \left[ \frac{(1+s)^2}{\gamma^2} - 1 \right] &= 1 \\ \frac{v^2}{\gamma^2} [1 + 2s + s^2 - \gamma^2] &= 1 \\ v^2 [1 + 2s + s^2 + s^2 - 1] &= 1 - s^2 \\ 2v^2 s(1+s) &= (1-s)(1+s) \\ \therefore 2v^2 &= \frac{1-s}{s} \end{aligned}$$

and so

$$u^2 + v^2 = 2v^2 + 1 = \frac{1}{s}. \quad (7.17)$$

Similarly the choice  $\frac{u}{v} = \frac{1-s}{\gamma}$  leads to

$$u^2 + v^2 = -\frac{1}{s}. \quad (7.18)$$

However, as we shall see shortly, this second choice is unphysical and will be discarded.

Hence

$$(c^+c + d^+d) + \gamma_k(c^+d^+ + cd) = \frac{1}{(u^2 + v^2)}(\alpha^+\alpha + \beta^+\beta - 2v^2)$$

and so the Hamiltonian (7.13) can be written

$$\mathcal{H} = E_N + JSv \sum_k \left[ \frac{1}{(u^2 + v^2)}(\alpha^+\alpha + \beta^+\beta) - 1 + s \right]. \quad (7.19)$$

Finally we write

$$\mathcal{H} = E_A + \sum_k \varepsilon_k (\alpha_k^+ \alpha_k + \beta_k^+ \beta_k) \quad (7.20)$$

where the energy of the excitations is

$$\varepsilon_k = JSv \frac{1}{(u^2 + v^2)} = JSvs = JSv \sqrt{1 - \gamma_k^2} \quad (7.21)$$

and

$$E_A = E_N - JSv \sum_k (1 - s) = - \frac{JNS(S+1)v}{2} + JSv \sum_k \sqrt{1 - \gamma_k^2} \quad (7.22)$$

We can now see that choosing the negative sign for  $u^2 + v^2$  as in (7.18) rather than the positive sign as in (7.17) would lead to negative excitation energies  $\varepsilon_k$ , and since the excitations are bosons we could obtain an arbitrarily low energy for the system by creating an arbitrary number of them.

The antiferromagnetic spin-waves we have obtained are doubly degenerate with energy  $JSv\sqrt{1 - \gamma_k^2}$ . The true result is triply degenerate since  $S_T = 1$  and there are three degenerate states with  $S_T^z = +1, 0, -1$ . The operator  $\alpha_k$  decreases  $S_T^z$  by one unit, while  $\beta_k$  increases it by one unit. There is no operator in spin-wave theory which creates an excitation with no change in  $S_T^z$ .

In the 1D case with  $S = \frac{1}{2}$  case the exact result for the energy of the excitations is known to be

$$\varepsilon_k = \frac{J\pi}{2} \sin k.$$

while the spin-wave result, using  $\gamma_k = \cos k$ ,  $S = \frac{1}{2}$ ,  $v = 2$ , has

$$\varepsilon_k = J\sqrt{1 - \cos^2 k} = J \sin k$$

i.e. of correct form but without the  $\frac{\pi}{2}$  factor. We also know that in the 1D,  $S = \frac{1}{2}$  case the ‘spin-wave spectrum’ is not a true branch, but rather the lower boundary of a continuum of states.

Nevertheless, even though the 1D,  $S = \frac{1}{2}$  case should be the most difficult since it shows the most extreme quantum effects, the results are rather good. For higher  $S$  and higher dimension the spin-wave results are even more satisfactory.

We can use our results (7.20), (7.21), and (7.22) to obtain an estimate of how different the energy of the true ground state is from that of the Néel state. The energy of the ground state is the value of (7.20) with  $\alpha_k^+ \alpha_k$  and  $\beta_k^+ \beta_k$  put to zero, since these operators count the number of *excited* bosons (spin-waves). This gives

$$E_A = E_N - \frac{NJv}{2}S + JSv \sum_k \sqrt{1 - \gamma_k^2}.$$

The sum over  $k$  can be converted to an integral which has the value  $\frac{2}{\pi} \times \frac{1}{2}$  in 1D and can be evaluated numerically in higher  $D$ . (The factor of  $\frac{1}{2}$  comes from the fact that the summation over  $k$  runs over  $\frac{N}{2}$  terms.) In 1D, for  $S = \frac{1}{2}$ , the result is

$$\frac{E_A}{N} = -0.75J + \frac{J}{\pi} \quad (\text{or } -0.431690J \text{ to 6 decimal places})$$

while the exact result is known to be  $-0.443147J$  (to 6 decimal places) which is in quite good agreement. (Note that the energy of the Néel state itself is  $\frac{E_N}{N} = -0.25$ , which is much less accurate!).

One can also calculate  $\langle S_j^z \rangle$  in the ground state in the SW approximation since  $S_j^z = S - a_j^+ a_j$  (for the up sublattice). This is done using the inverse Fourier transform  $\sum_j \langle a_j^+ a_j \rangle = \sum_k \langle c_k^+ c_k \rangle$ , the inverse of the Bogoliubov transformation  $c_k = u\alpha_k - v\beta_k^+$  and the fact that  $\langle \alpha_k^+ \alpha_k \rangle = \langle \beta_k^+ \beta_k \rangle = 0$  in the SW ground state.

Putting  $\langle \delta S_i^z \rangle = S - \langle S_i^z \rangle$ , then for  $S = \frac{1}{2}$  the results are

	$\langle \delta S_i \rangle$
3D (simple cubic)	0.078
2D (square)	0.20
1D	$\infty$

The result for 1D is clearly unphysical, and is associated with the fact that there is no long-range order. However for 2D and 3D the results are in quite good agreement with much more sophisticated calculations.

## References

1. Anderson, P.W.: Phys. Rev. **86**, 694 (1952) 77
2. Oguchi, T.: Phys. Rev. **117**, 117 (1960) 77