EFFECT OF NEXT NEAREST NEIGHBOURS INTERACTIONS ON TWO-MAGNON STATES OF THE HEISENBERG THREE-DIMENSIONAL FERROMAGNET*

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(Received November 18, 1977)

We consider a localized spin ferromagnet described by a Hamiltonian composed of single-ion anisotropy, quadratic and biquadratic (in spin operators) terms. Apart from the nearest neighbour, the other neighbour interactions are taken into account. A general secular equation which determines two-magnon bound state energies is found and analysed by means of group theory methods. Some computer results are given to illustrate the effect of next neighbour interactions on the two-magnon energy spectrum.

1. Introduction

Spin wave excitations in the Heisenberg model of ferromagnetism have been extensively studied [1, 2] for a long time. As long ago as 1931 Bethe [3] proved, for a chain of spins of magnitude $S = \frac{1}{2}$, that in the whole Brillouin zone there exist bound states of two spin waves, i. e. the states which have energy less than two free spin waves with the same total wave vector. The problem of bound states in the case of a three-dimensional model was first attacked by Dyson in 1956 who showed that they cannot exist in the center of the Brillouin zone [2].

In 1963 the problem under consideration was solved by Hanus [4] for a spin $S = \frac{1}{2}$ three-dimensional model and by Wortis [5] for both two- and three-dimensional models and an arbitrary spin. It was found that in the simple cubic nearest neighbour interaction Heisenberg model in the two-dimensional case, two-magnon bound states exist for any $\boldsymbol{K} \neq 0$, whereas in three dimensions there is a range of small $\boldsymbol{K}$ for which bound states do not exist; however they appear near the Brillouin zone boundary for $\boldsymbol{K}$ exceeding a threshold value.

* This work was supported by the Polish Academy of Sciences under project MR-I.9.

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In 1970 Silberglitt and Torrance [6] and Tonegawa [7] studied the effect of the single-ion anisotropy on the two-spin-wave bound state spectrum. They found that it causes the appearance of so-called "single-ion" bound states. Pink and Tremblay [8] and then Pink and Ballard [9] extended those considerations to the case when there are either isotropic or even anisotropic quadrupolar interactions.

There is still great interest in studying the problem of magnon bound states. The importance of the problem is due to the fact that the exsistence of magnon bound states imposes limits on the range of applicability of the linear or non-interacting spin-wave theory. Besides, multiple magnetic excitations were discovered experimentally in a simple spin system [10]. Various possibilities of experimental investigations of magnon pairing effects were reviewed in [11].

Recently the problem of the two-magnon bound states was solved for a non localized (itinerant) electron ferromagnet within the frame-work of a simple single-band Hubbard model [12, 13].

Up to now, to our knowledge, all the authors who studied the magnon bound state problem in three-dimensional models restricted themselves to the case of nearest neighbour interactions only.

Because of the relevance of the magnon bound states problem to the fundamentals of the spin wave theory, we find it interesting to complete the previous works by formulating the problem in the most general way in order to get solutions for any dimensionality and for interactions among neighbours from further coordination zones.

The organization of this paper is as follows. In Section II we derive the bound state condition from the Schrödinger equation. In Section III we analyse this condition by means of group theory methods for the case of a simple cubic lattice and two coordination zones. Section IV gives some exemplary numerical results. Finally in Section V we discuss the effect of next neighbour interactions on the two-magnon bound state spectrum.

2. *Problem formulation*

In the case of localized spin ferromagnets having the orbital angular momentum which is not quenched, non-bilinear or anisotropic terms in a spin Hamiltonian are believed to be of great importance.

Let our Hamiltonian contain long range spin interactions and be of the following form

$$H = -D\sum_j (S_j^z)^2 - \sum_n J_n \sum_{j,\vec{\delta}_n} \boldsymbol{S}_j \boldsymbol{S}_{j+\vec{\delta}_n} - \sum_n K_n \sum_{j,\vec{\delta}_n} (\boldsymbol{S}_j \boldsymbol{S}_{j+\vec{\delta}_n})^2, \tag{1}$$

where D is the single-ion anisotropy, J_n — the quadratic exchange interaction, K_n — the biquadratic exchange interaction, n indicates a coordination zone and $\vec{\delta}_n$ points to the lattice sites from the n-th coordination zone.

The one-magnon state can be written in the form

$$|\Psi_1\rangle = \sum_i c_i S_i^+ |0\rangle, \tag{2}$$

where $S_i^+ = S_i^x + iS_i^y$ is the spin operator which creates one spin deviation at site i, and $|0\rangle$ denotes the ferromagnetic ground state defined by

$$S_i^-|0\rangle = 0, \quad S_i^z|0\rangle = -S|0\rangle. \tag{3}$$

The operators obey the usual commutation relations

$$[S_i^+, S_{i'}^-] = 2S_i^z\delta_{ii'}, \quad [S_i^z, S_{i'}^\pm] = \pm S_i^\pm\delta_{ii'}. \tag{4}$$

The spin-wave energy spectrum may be easily computed from the Schrödinger equation

$$H|\Psi_1\rangle = E_1|\Psi_1\rangle. \tag{5}$$

The result reads

$$E_1(\boldsymbol{k}) = D(2S-1)+2S\sum_n [J_n+2S(S-1)K_n]\left[z_n - \sum_{\vec{\delta}_n}\cos \boldsymbol{k}\vec{\delta}_n\right] \tag{6}$$

with z_n being the number of neighbouring sites from the n-th coordination zone.

Now let us construct the wave-function $|\Psi_2\rangle$ of the two-magnon state in an analogous way

$$|\Psi_2\rangle = \sum_{il} \Phi(i, l)S_i^+ S_l^+|0\rangle \tag{7}$$

and look for solutions of

$$H|\Psi_2\rangle = E_2|\Psi_2\rangle. \tag{8}$$

To determine the two-magnon bound state energy spectrum we use a similar technique of calculations as that of [7] or [14]. After having introduced the centre of mass coordinates we get

$$\Phi(i, j) = \sum_{\boldsymbol{K}} \varphi_{\boldsymbol{K}}(\boldsymbol{r}_i - \boldsymbol{r}_j)\exp\left[i\boldsymbol{K}(\boldsymbol{r}_i + \boldsymbol{r}_j)\right] \tag{9}$$

$$(H_0 + V)\varphi_{\boldsymbol{K}}(\boldsymbol{R}) = E_2\varphi_{\boldsymbol{K}}(\boldsymbol{R}), \tag{10}$$

where

$$H_0\varphi_{\boldsymbol{K}}(\boldsymbol{R}) = 4S\sum_n [J_n+2S(S-1)K_n]\left[z_n\varphi_{\boldsymbol{K}}(\boldsymbol{R}) - \sum_{\vec{\delta}_n}\cos\frac{\boldsymbol{K}}{2}\vec{\delta}_n\varphi_{\boldsymbol{K}}(\boldsymbol{R}+\vec{\delta}_n)\right]. \tag{11}$$

$$V\varphi_{\boldsymbol{K}}(\boldsymbol{R}) = \Delta(\boldsymbol{R})\left\{-2D\varphi_{\boldsymbol{K}}(0)+4S(2S-1)\sum_n K_n\sum_{\vec{\delta}_n}\cos\tfrac{1}{2}\boldsymbol{K}\vec{\delta}_n\left[\varphi_{\boldsymbol{K}}(\vec{\delta}_n)\right.\right.$$

$$\left.\left.-\cos\frac{\boldsymbol{K}}{2}\vec{\delta}_n\varphi_{\boldsymbol{K}}(0)\right]\right\} + \Delta(\boldsymbol{R}-\vec{\delta}_n)\left\{-[2J_n+K_n(12S^2-12S+2)]\left[\varphi_{\boldsymbol{K}}(\vec{\delta}_n)\right.\right.$$

$$\left.\left.-\cos\frac{\boldsymbol{K}}{2}\vec{\delta}_n\varphi_{\boldsymbol{K}}(0)\right]\right\},$$

$$\boldsymbol{R} = 0, \{\vec{\delta}_1\}, \{\vec{\delta}_2\}, \ldots. \tag{12}$$

Above $\{\vec{\delta}_n\}$ means a set of z_n lattice vectors from the nth coordination zone, and $\Delta(\boldsymbol{R})$ equals 1 for $\boldsymbol{R}=0$ and vanishes for $\boldsymbol{R}\neq 0$.

If there were no magnon interactions ($V=0$), we would get immediately the obvious results

$$\varphi_{\boldsymbol{K}}(\boldsymbol{R}) = e^{i\boldsymbol{K}\boldsymbol{R}}, \tag{13}$$

and

$$E_2(\boldsymbol{K},\boldsymbol{k}) = E_1(\tfrac{1}{2}\boldsymbol{K}+\boldsymbol{k})+E_1(\tfrac{1}{2}\boldsymbol{K}-\boldsymbol{k}). \tag{14}$$

In order to solve the full equation (10) let us define a Green function

$$G_{\boldsymbol{K}}(\boldsymbol{R}) = \frac{1}{N}\sum_{\boldsymbol{k}}\frac{\cos \boldsymbol{k}\boldsymbol{R}}{E_2-E_2(\boldsymbol{K},\boldsymbol{k})} \tag{15}$$

which satisfies

$$H_0 G_{\boldsymbol{K}}(\boldsymbol{R})-E_2 G_{\boldsymbol{K}}(\boldsymbol{R}) = -\Delta(\boldsymbol{R}), \tag{16}$$

where N is the number of lattice sites in the crystal. We look for a solution in a form

$$\varphi_{\boldsymbol{K}}(\boldsymbol{R}) = \sum_{\boldsymbol{R}'} A_{\boldsymbol{K}}(\boldsymbol{R}')G_{\boldsymbol{K}}(\boldsymbol{R}-\boldsymbol{R}'). \tag{17}$$

By substituting (17) into (10) and by using (16) we find

$$A_{\boldsymbol{K}}(\boldsymbol{R}) = V\varphi_{\boldsymbol{K}}(\boldsymbol{R}). \tag{18}$$

Now we express the right-hand side of Eq. (18) in terms of the amplitudes $A_{\boldsymbol{K}}(\boldsymbol{R})$ using (12) and (17). In this way we find the set of $1+\sum_n z_n$ linear equations with respect to $A_{\boldsymbol{K}}(\boldsymbol{R})$.

The explicit form of the set reads

$$\begin{aligned}
&\left[1+\left(2d+\sum_{n'}U_{n'}\sum_{\vec{\delta}_{n'}}{}'\cos^2\frac{\boldsymbol{K}}{2}\vec{\delta}_{n'}\right)g_{\boldsymbol{K}}(0)-\sum_{n'}U_{n'}\sum_{\vec{\delta}_{n'}}{}'\cos\frac{\boldsymbol{K}}{2}\vec{\delta}_{n'}g_{\boldsymbol{K}}(\vec{\delta}_{n'})\right]A_{\boldsymbol{K}}(0)\\
&\quad+\sum_{n'}\sum_{\vec{\delta}_{n'}}{}'\left\{\left(2d+\sum_{n''}U_{n''}\sum_{\vec{\delta}_{n''}}{}'\cos^2\frac{\boldsymbol{K}}{2}\vec{\delta}_{n''}\right)g_{\boldsymbol{K}}(\vec{\delta}_{n'})\right.\\
&\quad-\tfrac{1}{2}\sum_{n''}U_{n''}\sum_{\vec{\delta}_{n''}}{}'\cos\frac{\boldsymbol{K}}{2}\vec{\delta}_{n''}[g_{\boldsymbol{K}}(\vec{\delta}_{n''}-\vec{\delta}_{n'})\\
&\quad\left.+g_{\boldsymbol{K}}(\vec{\delta}_{n''}+\vec{\delta}_{n'})]\right\}[A_{\boldsymbol{K}}(\vec{\delta}_{n'})+A_{\boldsymbol{K}}(-\vec{\delta}_{n'})] = 0,
\end{aligned} \tag{19a}$$

$$\begin{aligned}
&V_n\left[g_{\boldsymbol{K}}(\vec{\delta}_n)-\cos\frac{\boldsymbol{K}}{2}\vec{\delta}_n g_{\boldsymbol{K}}(0)\right]A_{\boldsymbol{K}}(0)\\
&\quad+V_n\sum_{n'}\sum_{\vec{\delta}_{n'}}{}'\left\{\tfrac{1}{2}[g_{\boldsymbol{K}}(\vec{\delta}_n-\vec{\delta}_{n'})+g_{\boldsymbol{K}}(\vec{\delta}_n+\vec{\delta}_{n'})]\right.\\
&\quad\left.-\cos\frac{\boldsymbol{K}}{2}\vec{\delta}_n g_{\boldsymbol{K}}(\vec{\delta}_{n'})\right\}[A_{\boldsymbol{K}}(\vec{\delta}_{n'})+A_{\boldsymbol{K}}(-\vec{\delta}_{n'})] = -A_{\boldsymbol{K}}(\vec{\delta}_n),
\end{aligned} \tag{19b}$$

where

$$U_n = 8S(2S-1)k_n, \quad V_n = 2j_n + k_n(12S^2 - 12S + 2),$$

$$j_n = J_n/J_1, \quad k_n = K_n/J_1, \quad d = D/J_1, \quad g_K(\boldsymbol{R}) = J_1 G_K(\boldsymbol{R}),$$

and $\sum'$ means the sum over the vectors $\vec{\delta}_n$ linearly independent on each other (inversion symmetry is assumed). It can be checked that the results of other authors are properly reproduced by the set (19) and correspond to an appropriate choice of the parameters (cf. [5–8]).

The effect of next nearest neighbour interactions was studied only in the case of a one-dimensional model [15–17].

The set of equations (19) makes it possible to test the effect of next (and even further) neighbour interactions on the two-magnon bound state not only for a spin chain but for two- and three-dimensional lattices as well.

3. Group theory analysis

As an example let us consider a simple cubic lattice with next nearest apart from nearest neighbour interactions. Then the vectors $\vec{\delta}_n$ take on the following values

$$\{\vec{\delta}_1\} = \pm a\boldsymbol{e}_1, \pm a\boldsymbol{e}_2, \pm a\boldsymbol{e}_3, \tag{20a}$$

$$\{\vec{\delta}_2\} = \pm a(\boldsymbol{e}_1+\boldsymbol{e}_2), \pm a(\boldsymbol{e}_1-\boldsymbol{e}_2), \pm a(\boldsymbol{e}_1+\boldsymbol{e}_3), \pm a(\boldsymbol{e}_3-\boldsymbol{e}_1), \pm a(\boldsymbol{e}_2+\boldsymbol{e}_3), \pm a(\boldsymbol{e}_3-\boldsymbol{e}_2) \tag{20b}$$

for the first and the second coordination zone, respectively, where a is the lattice constant and $\boldsymbol{e}_1$, $\boldsymbol{e}_2$, $\boldsymbol{e}_3$ are the basis versors.

Our detailed considerations will be carried out for the wave vector $\boldsymbol{K}$ oriented along the highest symmetry direction i. e. for $\boldsymbol{K} = K_x$ [1, 1, 1].

The problem is now of the order 19×19 ($z_1 = 6$, $z_2 = 12$), and the set of Eqs (19) may be written in a matrix form

$$\boldsymbol{M} \times \boldsymbol{A} = 0, \tag{21}$$

where

$$\boldsymbol{A}^+ = [|0\rangle, |1\rangle, |2\rangle, |3\rangle, \ldots, |17\rangle, |18\rangle],$$

$$|0\rangle = A_K(0), \quad |1\rangle = A_K(a\boldsymbol{e}_1), \quad |2\rangle = A_K(-a\boldsymbol{e}_1),$$

$$|3\rangle = A_K(a\boldsymbol{e}_2), \ldots, \quad |17\rangle = A_K(a(\boldsymbol{e}_3-\boldsymbol{e}_2)), \quad |18\rangle = A_K(-a(\boldsymbol{e}_3-\boldsymbol{e}_2)) \tag{22}$$

and the matrix elements M_{ij} are given in Appendix.

Eq. (21) has non-trivial solutions when the determinant of the matrix $\boldsymbol{M}$ vanishes.

Our aim is to find such a unitary matrix $\boldsymbol{U}$ which would transform $\boldsymbol{M}$ to a "block form". To achieve this we shall use the theory of point-group representations [18–20].

The matrix U operating on the set of the localized functions $|n\rangle$ ($n = 0, 1, \ldots, 18$) must transform it into the set of the symmetrized linear combinations $|\alpha, R(\alpha)\rangle$ which transform as bases of irreducible representations of the point-group under consideration.

$$|\alpha, R(\alpha)\rangle = \sum_{l=0}^{18} U(l; \alpha, R(\alpha))\,|l\rangle, \tag{23}$$

where α specifies an irreducible representation according to which a given symmetrized combination transforms, and $R(\alpha)$ enumerates those symmetrized combinations.

It follows from (22), (18) and (12) that for $\boldsymbol{K} = K_x\,[1, 1, 1]$ only these of the functions $|n\rangle$ can transform into themselves which, as it is shown in Fig. 1, are marked with the

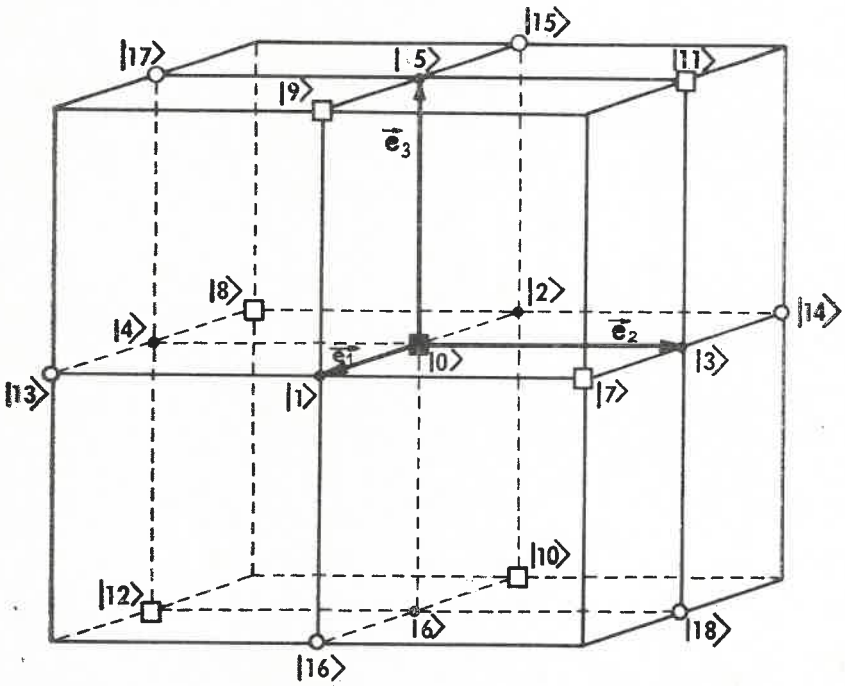

Fig. 1. Symmetries of the localized functions $|n\rangle$ for the s. c. lattice and $\boldsymbol{K} = K_x\,[1, 1, 1]$

same pattern. All the symmetry operations which leave the set of the functions $|n\rangle$ unchanged form the group D_{3d}. This group consists of 6 classes. Using the character table we have decomposed a reducible representation Γ of the group D_{3d} into the irreducible ones

$$\Gamma = 4\Gamma_1 + 3\Gamma_{12} + \Gamma_1' + 2\Gamma_2' + 3\Gamma_{12}', \tag{24}$$

where Bouckaert, Smoluchowski and Wigner's nomenclature is adopted. The representations Γ_{12} and Γ_{12}' are two-dimensional, the others are one-dimensional.

After having found the irreducible representations, we determine the symmetrized functions $|\alpha, R(\alpha)\rangle$ which transform according to them (see Appendix of [18] for a detailed

description of similar considerations). The unitary matrix U can now be easily constructed by forming its columns from the symmetrized functions. The final result is

$$U = \begin{array}{|cccccccccccccccccc|}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & a & 0 & 0 & b & 0 & 0 & c & 0 & 0 & 0 & a & 0 & c & 0 & 0 & -b & 0 & 0 \\
0 & a & 0 & 0 & b & 0 & 0 & c & 0 & 0 & 0 & -a & 0 & -c & 0 & 0 & b & 0 & 0 \\
0 & a & 0 & 0 & -b & 0 & 0 & c & 0 & 0 & 0 & a & 0 & c & 0 & 0 & b & 0 & 0 \\
0 & a & 0 & 0 & -b & 0 & 0 & c & 0 & 0 & 0 & -a & 0 & -c & 0 & 0 & -b & 0 & 0 \\
0 & a & 0 & 0 & 0 & 0 & 0 & -d & 0 & 0 & 0 & a & 0 & -d & 0 & 0 & 0 & 0 & 0 \\
0 & a & 0 & 0 & 0 & 0 & 0 & -d & 0 & 0 & 0 & -a & 0 & d & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & a & 0 & 0 & 0 & 0 & 0 & d & 0 & 0 & 0 & a & 0 & -d & 0 & 0 & 0 & 0 \\
0 & 0 & a & 0 & 0 & 0 & 0 & 0 & d & 0 & 0 & 0 & -a & 0 & d & 0 & 0 & 0 & 0 \\
0 & 0 & a & 0 & 0 & b & 0 & 0 & -c & 0 & 0 & 0 & a & 0 & c & 0 & 0 & b & 0 \\
0 & 0 & a & 0 & 0 & b & 0 & 0 & -c & 0 & 0 & 0 & -a & 0 & -c & 0 & 0 & -b & 0 \\
0 & 0 & a & 0 & 0 & -b & 0 & 0 & -c & 0 & 0 & 0 & a & 0 & c & 0 & 0 & -b & 0 \\
0 & 0 & a & 0 & 0 & -b & 0 & 0 & -c & 0 & 0 & 0 & -a & 0 & -c & 0 & 0 & b & 0 \\
0 & 0 & 0 & a & 0 & 0 & 0 & 0 & 0 & d & a & 0 & 0 & 0 & 0 & 0 & 0 & 0 & d \\
0 & 0 & 0 & a & 0 & 0 & 0 & 0 & 0 & d & -a & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -d \\
0 & 0 & 0 & a & 0 & 0 & b & 0 & 0 & -c & a & 0 & 0 & 0 & 0 & b & 0 & 0 & -c \\
0 & 0 & 0 & a & 0 & 0 & b & 0 & 0 & -c & -a & 0 & 0 & 0 & 0 & -b & 0 & 0 & c \\
0 & 0 & 0 & a & 0 & 0 & -b & 0 & 0 & -c & -a & 0 & 0 & 0 & 0 & b & 0 & 0 & c \\
0 & 0 & 0 & a & 0 & 0 & -b & 0 & 0 & -c & a & 0 & 0 & 0 & 0 & -b & 0 & 0 & -c \\
\end{array} \qquad (25)$$

Γ_1 Γ_{12} Γ'_1 Γ'_2 Γ'_{12}

where $a = 1/\sqrt{6}$, $b = 1/2$, $c = 1/\sqrt{12}$, $d = 1/\sqrt{3}$.

This matrix reduces M to a block diagonal form

$$U^+MU = \begin{bmatrix} F_1 & & & \\ & F_2 & & \\ & & F_2 & \\ & & & E \end{bmatrix}, \qquad (26)$$

where E is a 9×9 unitary matrix and

$$F_1 = \begin{bmatrix} M_{00} & \sqrt{6}\,M_{01} & \sqrt{6}\,M_{07} & \sqrt{6}\,M_{0,13} \\ \sqrt{6}\,M_{10} & M_{11}+M_{12}+4M_{13} & 2M_{1,11}+4M_{17} & 2M_{1,17}+4M_{1,13} \\ \sqrt{6}\,M_{70} & 2M_{75}+4M_{71} & M_{77}+M_{78}+4M_{79} & 2M_{7,13}+4M_{7,15} \\ \sqrt{6}\,M_{13,0} & 2M_{13,5}+4M_{13,1} & 2M_{13,7}+4M_{13,9} & M_{13,13}+M_{13,14}+4M_{13,15} \end{bmatrix} \qquad (27)$$

$$\boldsymbol{F}_2 = \begin{bmatrix} M_{11}+M_{12}-2M_{13} & 2M_{17}-2M_{1,11} & 2M_{1,13}-2M_{1,17} \\ 2M_{71}-2M_{75} & M_{77}+M_{78}-2M_{79} & 2M_{7,13}-2M_{7,15} \\ 2M_{13,1}-2M_{13,5} & 2M_{13,7}-2M_{13,9} & M_{13,13}+M_{13,14}-2M_{13,15} \end{bmatrix}. \quad (28)$$

It follows from (26) that (similarly as if there were no next nearest neighbour interactions) there are only two conditions which determine the two-magnon bound state energies: one for the singly degenerate (s-wave) states and the other for the doubly degenerate (d-wave) states. The modes of Γ_1', Γ_2' and Γ_{12}' symmetries are absent. Eqs. (26), (27) and (28) are the main result of the present paper. In the case when the next nearest neighbours effect is neglected our results become identical as those of Pink and Tremblay [8], obtained by a different method.

4. *Numerical results*

Our aim now is to find the energy of two-magnon bound states from the equations

$$\det(\boldsymbol{F}_1) = 0 \quad (29a)$$

and

$$\det(\boldsymbol{F}_2) = 0. \quad (29b)$$

The matrix elements which enter into (27) and (28) contain the following parameters: d, j_2, k_1 and k_2.

These parameters should be chosen in such a way so that the single magnon spectrum (6) is stable i. e. $E(\boldsymbol{k})$ has a minimum for $\boldsymbol{k} = 0$. From this requirement we get (cf. [17])

$$1+2S(S-1)k_1+4[j_2+2S(S-1)k_2] > 0. \quad (30)$$

We shall illustrate the solutions of Eqs. (29) considering a specific choice of parameters, namely

$$d = k_1 = k_2 = 0, \quad S = 1, \quad j_2 > -1/4. \quad (31)$$

Solutions of (29) which correspond to the two-magnon bound state energies are looked for outside of the two-magnon band. The band is bounded by (see (14) and (6))

$$\varepsilon_{\min}(\boldsymbol{K}) = \min_{\boldsymbol{k}} E_2(\boldsymbol{K}, \boldsymbol{k}) \quad \text{and} \quad \varepsilon_{\max}(\boldsymbol{K}) = \max_{\boldsymbol{k}} E_2(\boldsymbol{K}, \boldsymbol{k}) \quad (32)$$

The extrema (32) depend strongly on j_2 and are

(a) $-\frac{1}{4} \leqslant j_2 < 0$

$$\varepsilon_{\min}(\boldsymbol{K}) = \begin{cases} \varepsilon_1 & \text{for} \quad 0 \leqslant X \leqslant X_1, \\ \varepsilon_2 & \text{for} \quad X_1 \leqslant X \leqslant \pi, \end{cases}$$

$$\varepsilon_{\max}(\boldsymbol{K}) = \begin{cases} \varepsilon_3 & \text{for} \quad 0 \leqslant X \leqslant X_2, \\ \varepsilon_4 & \text{for} \quad X_2 \leqslant X \leqslant \pi, \end{cases} \quad (33a)$$

(b) $j_2 = 0$

$$\varepsilon_{\min}(\boldsymbol{K}) = \varepsilon_1, \quad \varepsilon_{\max}(\boldsymbol{K}) = \varepsilon_3, \quad (33b)$$

(c) $0 < j_2 \leqslant \frac{1}{4}$

$$\varepsilon_{\min}(K) = \begin{cases} \varepsilon_1 & \text{if} \quad 0 \leqslant X \leqslant X_2, \\ \varepsilon_6 & \text{if} \quad X_2 \leqslant X \leqslant \pi, \end{cases}$$

$$\varepsilon_{\max}(K) = \begin{cases} \varepsilon_3 & \text{if} \quad 0 \leqslant X \leqslant X_1, \\ \varepsilon_5 & \text{if} \quad X_1 \leqslant X \leqslant \pi, \end{cases} \tag{33c}$$

(d) $\frac{1}{4} \leqslant j_2$

$$\varepsilon_{\min}(K) = \begin{cases} \varepsilon_1 & \text{if} \quad 0 \leqslant X \leqslant X_2, \\ \varepsilon_6 & \text{if} \quad X_2 \leqslant X \leqslant \pi, \end{cases}$$

$$\varepsilon_{\max}(K) = \varepsilon_5, \tag{33d}$$

where

$$X = K_x a,$$

$$X_1 = 2 \arccos\left[\frac{1}{4|j_2|} - \tfrac{1}{2}\left(\frac{1}{4j_2^2} - 4\right)^{1/2}\right],$$

$$X_2 = 2 \arccos\left[-\frac{1}{16|j_2|} + \tfrac{1}{2}\left(\frac{1}{64j_2^2} + 2\right)^{1/2}\right].$$

$$\varepsilon_1 = 24\left(1 - \cos\frac{X}{2}\right) + 24j_2(1 - \cos X),$$

$$\varepsilon_2 = 24 - 64|j_2| - 8\cos\frac{X}{2} - \frac{4}{|j_2|}\cos^2\frac{X}{2} + 16|j_2|\cos^2\frac{X}{2} + 16\cos^3\frac{X}{2} - 16|j_2|\cos^4\frac{X}{2},$$

$$\varepsilon_3 = 24\left(1 + \cos\frac{X}{2}\right) + 24j_2(1 - \cos X),$$

$$\varepsilon_4 = 24(1 - |j_2| - |j_2|\cos X) - \frac{3}{|j_2|}\frac{\cos^2\frac{X}{2}}{\cos X},$$

$$\varepsilon_5 = 48 - \varepsilon_2,$$

$$\varepsilon_6 = 48 - \varepsilon_4.$$

The results of numerical computations are plotted in Fig. 2. It shows that when j_2 increases the whole energy spectrum moves upwards. The question arises whether there is any threshold value of j_2 for which the magnon bound states would not exist below the band any longer. To make this point clear we have computed the two-magnon bound state energies at the Brillouin zone boundary $\left(\text{i. e. for } K_x = \frac{\pi}{a}\right)$ vs. j_2. In this case we get

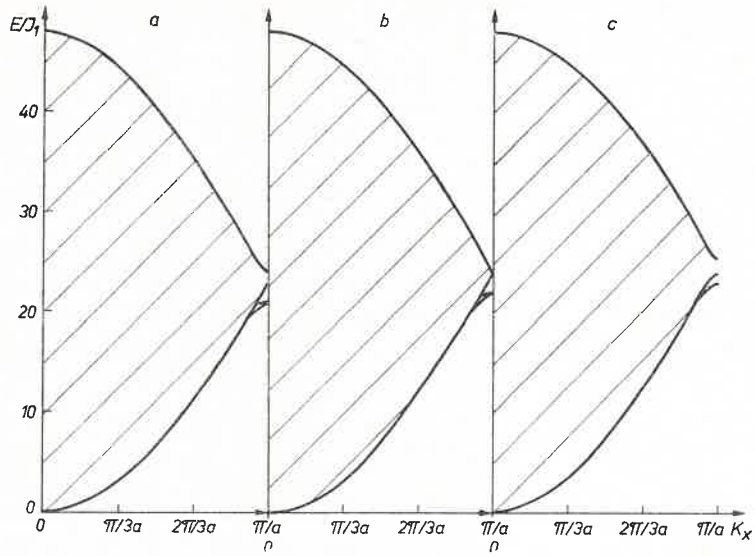

Fig. 2. The energies of two-magnon bound states for a s. c. lattice with $S = 1$ and (a) $j_2 = -0.02$, (b) $j_2 = 0$, (c) $j_2 = 0.02$. The upper curve is doubly degenerate (d-wave) and the lower one is non-degenerate (s-wave). Hatched area is the two-magnon band

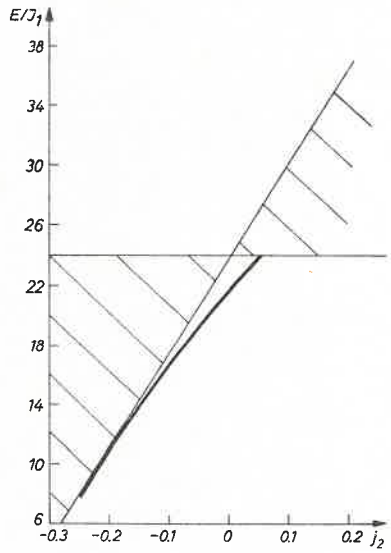

Fig. 3. Bound state energies with $\boldsymbol{K} = \frac{\pi}{a}$ [1, 1, 1] versus j_2

solutions which are three-fold degenerated ($\boldsymbol{F}_2$ itself is doubly degenerate). This solution moves more and more close to the band when $|j_2|$ increases and disapears for a threshold value $j_{2c} = 0.05$. This behaviour is shown in Fig. 3.

5. *Conclusions*

We have calculated the effect of next nearest neighbour exchange interactions upon the two-magnon bound states of an three-dimensional Heisenberg ferromagnet. Using an equation of motion mthod we have found a general secular equation which determines the two-magnon bound states energy spectrum. The equation has been analysed by means of group theory methods. We have shown that for a simple cubic lattice there are two types of solutions corresponding to *s*-wave states and *d*-wave states (doubly degenerated) respectively. Detailed numerical calculations have been carried out, in accordance with the practice of other authors, for a wave vector $\boldsymbol{K}$ in the [111] direction. The parameters were chosen from the range within which the ground state may be assumed to be fully aligned. The principal result which has come out of this work is the observation that the next nearest neighbour exchange interactions have very strong effect on the behaviour of the two-magnon bound states. This effect becomes drastic and makes the two-magnon bound states vanish, when the next nearest neighbour exchange parameter reaches a value of 5% of the nearest neighbour exchang parameter.

The author wants to give special thanks to Professor J. Morkowski for bringing this problem to his attention.

APPENDIX

The matrix elements M_{ij} for a simple cubic lattice are listed below. In the case when two coordination zones are taken into account the matrix $\boldsymbol{M}$ is of the order of 19×19. For the wave vector $\boldsymbol{K}$ lying in the [111] direction there are only 28 different matrix elements, they are:

$$M_{00} = 1+2dg_1-3U_1c(g_2-cg_1)-3U_2C(g_4-Cg_1)-3U_2(g_5-g_1),$$

$$M_{01} = M_{02} = M_{03} = M_{04} = M_{05} = M_{06} = 2dg_2-U_1c(g_3+2g_6-3cg_2)-U_2 \times[C(2g_7+g_9-3Cg_2)+2g_8+g_{10}-3g_2],$$

$$M_{07} = M_{08} = M_{09} = M_{0,10} = M_{0,11} = M_{0,12} = 2dg_4-U_1c(g_9+2g_7-3cg_4) -U_2[C(2g_{14}+g_{11}-3Cg_4)+2g_{15}+g_{13}-3g_4],$$

$$M_{0,13} = M_{0,14} = M_{0,15} = M_{0,16} = M_{0,17} = M_{0,18} = 2dg_5-U_1c(g_{10}+2g_8 -3cg_5)-U_2[C(2g_{15}+g_{13}-3Cg_5)+2g_{16}+g_{12}-3g_5],$$

$$M_{10} = M_{20} = M_{30} = M_{40} = M_{50} = M_{60} = V_1(g_2-cg_1),$$

$$M_{70} = M_{80} = M_{90} = M_{10,0} = M_{11,0} = M_{12,0} = V_2(g_4-Cg_1),$$

$$M_{13,0} = M_{14,0} = M_{15,0} = M_{16,0} = M_{17,0} = M_{18,0} = V_2(g_5 - g_1),$$

$$M_{11} = M_{22} = M_{33} = M_{44} = M_{55} = M_{66} = 1 + V_1(g_3 - cg_2),$$

$$M_{77} = M_{88} = M_{99} = M_{10,10} = M_{11,11} = M_{12,12} = 1 + V_2(g_{11} - Cg_4),$$

$$M_{13,13} = M_{14,14} = M_{15,15} = M_{16,16} = M_{17,17} = M_{18,18} = 1 + V_2(g_{12} - g_5),$$

$$M_{12} = M_{34} = M_{56} = M_{21} = M_{43} = M_{65} = V_1(g_3 - cg_2),$$

$$M_{78} = M_{9,10} = M_{11,12} = M_{87} = M_{10,9} = M_{12,11} = V_2(g_{11} - Cg_4),$$

$$M_{13,14} = M_{14,13} = M_{15,16} = M_{16,15} = M_{17,18} = M_{18,17} = V_2(g_{12} - g_5),$$

$$M_{13} = M_{24} = M_{35} = M_{46} = M_{31} = M_{42} = M_{53} = M_{64} = M_{15} = M_{26} = M_{51}$$
$$= M_{62} = M_{14} = M_{25} = M_{16} = M_{36} = M_{45} = M_{41} = M_{61} = M_{52} = M_{63} = M_{54}$$
$$= M_{23} = M_{32} = V_1(g_6 - cg_2),$$

$$M_{17} = M_{19} = M_{28} = M_{2,10} = M_{37} = M_{3,11} = M_{48} = M_{4,12} = M_{59} = M_{5,11}$$
$$= M_{6,10} = M_{6,12} = M_{18} = M_{27} = M_{38} = M_{47} = M_{5,12} = M_{6,11} = M_{1,10}$$
$$= M_{29} = M_{3,12} = M_{4,11} = M_{5,10} = M_{69} = V_1(g_7 - cg_4),$$

$$M_{1,11} = M_{1,12} = M_{2,11} = M_{2,12} = M_{39} = M_{3,10} = M_{49} = M_{4,10} = M_{57}$$
$$= M_{58} = M_{67} = M_{68} = V_1(g_9 - cg_4),$$

$$M_{1,13} = M_{1,14} = M_{1,15} = M_{1,16} = M_{2,13} = M_{2,14} = M_{2,15} = M_{2,16}$$
$$= M_{3,13} = M_{3,14} = M_{3,17} = M_{3,18} = M_{4,13} = M_{4,14} = M_{4,17} = M_{4,18}$$
$$= M_{5,15} = M_{5,16} = M_{5,17} = M_{5,18} = M_{6,15} = M_{6,16} = M_{6,17}$$
$$= M_{6,18} = V_1(g_8 - cg_5),$$

$$M_{1,17} = M_{1,18} = M_{2,17} = M_{2,18} = M_{3,15} = M_{3,16} = M_{4,15} = M_{4,16}$$
$$= M_{5,13} = M_{5,14} = M_{6,13} = M_{6,14} = V_1(g_{10} - cg_5),$$

$$M_{79} = M_{7,10} = M_{89} = M_{8,10} = M_{9,11} = M_{9,12} = M_{10,12} = M_{7,11} = M_{10,11}$$
$$= M_{7,12} = M_{8,11} = M_{8,12} = M_{97} = M_{10,7} = M_{98} = M_{10,8} = M_{11,9} = M_{12,9}$$
$$= M_{11,10} = M_{12,10} = M_{11,7} = M_{12,7} = M_{11,8} = M_{12,8} = V_2(g_{14} - Cg_4),$$

$$M_{7,13} = M_{7,14} = M_{8,13} = M_{8,14} = M_{9,15} = M_{9,16} = M_{10,15} = M_{10,16}$$
$$= M_{11,17} = M_{11,18} = M_{12,17} = M_{12,18} = V_2(g_{13} - Cg_5),$$

$$M_{7,15} = M_{7,16} = M_{7,17} = M_{7,18} = M_{8,15} = M_{8,16} = M_{8,17} = M_{8,18}$$
$$= M_{9,13} = M_{9,14} = M_{9,17} = M_{9,18} = M_{10,13} = M_{10,14} = M_{10,17} = M_{10,18}$$
$$= M_{11,13} = M_{11,14} = M_{11,15} = M_{11,16} = M_{12,13} = M_{12,14} = M_{12,15}$$
$$= M_{12,16} = V_2(g_{15} - Cg_5).$$

$$M_{71} = M_{72} = M_{73} = M_{74} = M_{81} = M_{82} = M_{83} = M_{84} = M_{91} = M_{92} = M_{95}$$
$$= M_{96} = M_{10,1} = M_{10,2} = M_{10,5} = M_{10,6} = M_{11,3} = M_{11,4} = M_{11,5}$$
$$= M_{11,6} = M_{12,3} = M_{12,4} = M_{12,5} = M_{12,6} = V_2(g_7 - Cg_2),$$

$$M_{75} = M_{76} = M_{85} = M_{93} = M_{94} = M_{10,3} = M_{10,4} = M_{11,1} = M_{11,2} = M_{86}$$
$$= M_{12,1} = M_{12,2} = V_2(g_9 - Cg_2),$$

$$M_{13,1} = M_{13,2} = M_{13,3} = M_{13,4} = M_{14,1} = M_{14,2} = M_{14,3} = M_{14,4}$$
$$= M_{15,1} = M_{15,2} = M_{15,5} = M_{15,6} = M_{16,1} = M_{16,2} = M_{16,5} = M_{16,6}$$
$$= M_{17,3} = M_{17,4} = M_{17,5} = M_{17,6} = M_{18,3} = M_{18,4} = M_{18,5} = M_{18,6}$$
$$= V_2(g_8 - g_2).$$

$$M_{13,5} = M_{13,6} = M_{14,5} = M_{14,6} = M_{15,3} = M_{15,4} = M_{16,3} = M_{16,4}$$
$$= M_{17,1} = M_{17,2} = M_{18,1} = M_{18,2} = V_2(g_{10} - g_2),$$

$$M_{13,7} = M_{18,8} = M_{14,7} = M_{14,8} = M_{15,9} = M_{15,10} = M_{16,9} = M_{16,10}$$
$$= M_{17,11} = M_{17,12} = M_{18,11} = M_{18,12} = V_2(g_{13} - g_4),$$

$$M_{13,9} = M_{13,10} = M_{13,11} = M_{13,12} = M_{14,9} = M_{14,10} = M_{14,11}$$
$$= M_{14,12} = M_{15,7} = M_{15,8} = M_{15,11} = M_{15,12} = M_{16,7} = M_{16,8} = M_{16,11}$$
$$= M_{16,12} = M_{17,7} = M_{17,8} = M_{17,9} = M_{17,10} = M_{18,7} = M_{18,8} = M_{18,9}$$
$$= M_{18,10} = V_2(g_{15} - g_4),$$

$$M_{13,15} = M_{13,16} = M_{13,17} = M_{13,18} = M_{14,15} = M_{14,16} = M_{14,17}$$
$$= M_{14,18} = M_{15,17} = M_{15,18} = M_{16,17} = M_{16,18} = M_{15,13} = M_{16,13}$$
$$= M_{17,13} = M_{18,13} = M_{15,14} = M_{16,14} = M_{17,14} = M_{18,14} = M_{17,15}$$
$$= M_{18,15} = M_{17,16} = M_{18,16} = V_2(g_{16} - g_5),$$

where

$$c = \cos(K_x a/2), \quad C = \cos(K_x a),$$

$$g_1 = 1/N \sum_k 1/W,$$

$$g_2 = 1/N \sum_k \cos k_x a/W,$$

$$g_3 = 1/N \sum_k \cos^2 k_x a/W,$$

$$g_4 = 1/N \sum_k \cos (k_x+k_y)a/W,$$

$$g_5 = 1/N \sum_k \cos (k_x-k_y)a/W,$$

$$g_6 = 1/N \sum_k \cos k_x a \cos k_y a/W,$$

$$g_7 = 1/N \sum_k \cos k_x a \cos (k_x+k_y)a/W,$$

$$g_8 = 1/N \sum_k \cos k_x a \cos (k_x-k_y)a/W,$$

$$g_9 = 1/N \sum_k \cos k_x a \cos (k_y+k_z)a/W,$$

$$g_{10} = 1/N \sum_k \cos k_x a \cos (k_y-k_z)a/W,$$

$$g_{11} = 1/N \sum_k \cos^2 (k_x+k_y)a/W,$$

$$g_{12} = 1/N \sum_k \cos^2 (k_x-k_y)a/W,$$

$$g_{13} = 1/N \sum_k \cos (k_x+k_y)a \cos (k_x-k_y)a/W,$$

$$g_{14} = 1/N \sum_k \cos (k_x+k_y)a \cos (k_x+k_z)a/W,$$

$$g_{15} = 1/N \sum_k \cos (k_x+k_y)a \cos (k_x-k_z)a/W,$$

$$g_{16} = 1/N \sum_k \cos (k_x-k_y)a \cos (k_x-k_z)a/W,$$

and

$$W = E_2/J_1 - 2d(2S-1) + 8S[1+2S(S-1)k_1]\,[(\cos k_x a + \cos k_y a + \cos k_z a) \times \cos (K_x a/2) - 3] + 8S[j_2 + 2S(S-1)k_2]\,\{[\cos (k_x+k_y)a + \cos (k_x+k_z)a + \cos (k_y+k_z)a] \cos K_x a + \cos (k_x-k_y)a + \cos (k_x-k_z)a + \cos (k_y-k_z)a - 6\}.$$

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