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Three-magnon bound states in an $S=1$ linear chain with next-nearest-neighbour interaction

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Abstract. The problem of three spin deviations from a fully aligned state is studied for the Heisenberg model with next-nearest-neighbour interactions for the case of spin 1. The method used is a straightforward generalization of the equation-of-motion method of Fukuda and Wortis, taking care of the unphysical states. The resulting integral equation is solved in one dimension and the dependence of the bound states on the next-nearest-neighbour interaction discussed. Numerical calculations have also been done for closed chains containing up to 40 spins. By using C_N invariance of the Hamiltonian, the dimensionality of the space is substantially reduced. The results of the finite-chain calculation agree well with solutions obtained from the equation-of-motion method.

1. Introduction

The Heisenberg chain of spin-$\frac{1}{2}$ particles has been of considerable interest in recent years. The ground state of the Heisenberg Hamiltonian

$$H = -\frac{1}{2}J\sum_i \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}$$

with $J > 0$ is the state of completely aligned spins while the first excited state is the spin-wave state. Interest in the higher excited states, consisting of bound states of two reversed spins arose due to the observation of bound-state complexes of excitations in one-dimensional magnon systems [1]. Theoretically, the existence of bound states in the Heisenberg system was established by the pioneering work of Hanus [2], Fukuda and Wortis [3], and Wortis [4]. Majumdar [5] investigated the dependence of these bound states on the strength of the next-nearest-neighbour interactions and had studied the first two excited states of the Hamiltonian

$$H = -\tfrac{1}{2}J\sum_i \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} - \tfrac{1}{2}J\alpha\sum_i \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2}. \tag{1}$$

Ghosh and Mukhopadhyay [6] had extended these results to higher dimensions. It was found that as α increases, the bound states merge into the continuum.

Theoretical interest in the next excited state of three reversed spins has been rather subdued due to mathematical complexities. For the spin-$\frac{1}{2}$ case, Bethe [7] had pointed out that in addition to the spin-wave solutions, bound complexes of reversed spins propagate through the lattice. Bethe's method is difficult to generalize to higher

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dimensions and subsequent efforts have been generally confined to lower excited states. Majumdar [8] used Faddeev's technique [9] to treat the three-spin deviation problem for the spin-$\frac{1}{2}$ case. In this work Majumdar used the Dyson Hamiltonian [10] of ideal bosonic spin waves instead of considering the spin operators themselves. The disadvantage of this Hamiltonian is that it does not reproduce the kinematical constraint of the impossibility of two spin reversals at the same site and leads to unphysical bound states, in addition to the real ones. However these unphysical bound states are relatively easy to identify and the formalism leads to simple Faddeev equations. Himbergen [11] succeeded in obtaining the Faddeev equations for the three-magnon T-matrix of the Heisenberg spin Hamiltonian. Himbergen's method rigorously takes into account the kinematical constraints mentioned above, though it leads to considerable difficulties with the Faddeev equations.

In this work, we consider a linear chain of spin-one Heisenberg ferromagnets with next-nearest-neighbour interactions. For the spin-one case there are some additional features which do not exist for the spin-$\frac{1}{2}$ case. There can now be two spin reversals at the same site. The bound complexes of three reversals can be of two types: (i) in which two spin reversals at one site are coupled with a single reversal at a different site, and (ii) in which the three spin reversals are all at different sites like the spin-$\frac{1}{2}$ case. Unphysical states also continue to appear here except that these are caused by three spin reversals at the same site.

2. One- and two-magnon subspace

In the following, we follow Fukuda and Wortis [3] and write down the wave equations for the n-spin deviation subspace. For the Hamiltonian (1), the fully aligned state, denoted by $|0\rangle$ is the ground state for $J > 0$ and $\alpha > 0$ with an energy $E_0 = -NJS^2(1+\alpha)$. The wavefunction for the one-magnon subspace is written as

$$\Psi_1 = \sum_{i=1}^{N} U(i) S_i^+ |0\rangle. \tag{2}$$

One can explicitly write down and solve the Schrodinger equation and obtain the spin-wave excitation energy as

$$\omega(k) = E - E_0 = 2SJ(1+\alpha) - 2SJ\cos(ka) - 2SJ\alpha\cos(2ka) \tag{3}$$

where a is the lattice spacing.

For the case of two spin deviations, following Fukuda and Wortis [3], the wavefunction can be written as

$$\Psi_2 = \sum_{i,j=1}^{N} U(i,j) S_i^+ S_j^+ |0\rangle. \tag{4}$$

The wave equation can be written as

$$\omega\Psi_2 = \sum_{i,j=1}^{N} U(i,j)[H, S_i^+ S_j^+]|0\rangle. \tag{5}$$

The commutator in equation (5) can be explicitly calculated for the Hamiltonian (1) and one gets

$$\begin{aligned}[\omega - 4JS(1+\alpha)]U(i,j) = -JS\Big[&\sum_{l=\pm1}\{U(i+l,j)+U(i,j+l)\} \\ &+ \alpha\sum_{l=\pm1}\{U(i+2l,j)+U(i,j+2l)\}\Big] \\ &+ \tfrac{1}{2}\sum_{l=\pm1}\delta_{i,j+l}\{U(i,i)+U(j,j)-2U(i,j)\} \\ &+ \frac{\alpha}{2}\sum_{l=\pm1}\delta_{i,j+2l}\{U(i,i)+U(j,j)-2U(i,j)\}. \end{aligned} \tag{6}$$

For spin-$\frac{1}{2}$, the amplitudes $U(i,i)$ are unphysical and have to be defined artificially by extending the expression for $U(i,j)$ for $i \neq j$ to be valid for $i = j$. For $S = 1$ however no such problem arises.

Using the centre-of-mass coordinate system and Fourier transform, equation (6) becomes

$$[\omega - E_K(k)]U_K(k) = \frac{1}{N}\sum_{k'\in F} V_K(k,k')\,U_K(k') \tag{7}$$

where F is reciprocal lattice. $E_K(k)$ is the energy of two free spin waves, given by

$$E_K(k) = 4JS[1+\alpha-\cos(Ka/2)\cos(ka)-\alpha\cos(Ka)\cos(2ka)]. \tag{8}$$

The interaction $V_K(k,k')$ is given by

$$\begin{aligned} V_K(k,k') = 2J[&\cos(ka)(\cos(Ka/2)-\cos(k'a)) \\ &+ \alpha\cos(2ka)(\cos(Ka)-\cos(2k'a))]. \end{aligned} \tag{9}$$

Equation (9) has been studied and conditions for the existence of bound states are obtained as a function of the relative strength α.

3. Three-magnon case

In the three-spin deviation case, the wave equation can be simplified using the symmetry properties of the amplitudes as shown by Millet and Kaplan [12]. For convenience the Hamiltonian will be written as

$$H = -\tfrac{1}{2}\sum_{i,j=1}^{N} J(i,j)\,\boldsymbol{S}_i\cdot\boldsymbol{S}_j \tag{10}$$

where

$$J(i,j) = \begin{cases} J & \text{if } i = j\pm1 \\ \alpha J & \text{if } i = j\pm2 \\ 0 & \text{otherwise.} \end{cases} \tag{11}$$

The wavefunction in the three-magnon subspace is given by

$$\Psi_3 = \sum_{j,k,l=1}^{N} U(j,k,l) S_j^+ S_k^+ S_l^+ |0\rangle. \tag{12}$$

The amplitude $U(j,k,l)$ is invariant with respect to any permutation of j, k, and l. The wave equation is

$$\omega\Psi_3 = \sum_{j,k,l=1}^{N} U(j,k,l)\left[H, S_j^+ S_k^+ S_l^+\right]|0\rangle. \tag{13}$$

the commutator in (13) is given by

$$\begin{aligned}\left[H, S_j^+ S_k^+ S_l^+\right] = \sum_{CP}\Big\{ S_j^+ S_k^+ \left[H, S_l^+\right] + S_k^+ \left[\left[H, S_j^+\right], S_l^+\right]\Big\} \\ + \left[\left[\left[H, S_j^+\right], S_k^+\right], S_l^+\right]\end{aligned} \tag{14}$$

where CP stands for cyclic permutation.

The first term in the RHS of equation (14) describes the motion of free spin waves. The second term represents the interaction between two spin waves. The third term, which is a three-body interaction, vanishes for the Hamiltonian (1).

The equations determining the amplitudes can be obtained in a straightforward manner and are given by

$$\begin{aligned}\omega U(j,k,l) = 2S \sum_{CP,i} J(l,i)\left[U(j,k,l) - U(j,k,i)\right] \\ + \sum_{CP} J(k,j)\left[U(j,j,l) + U(k,k,l) - 2U(j,k,l)\right].\end{aligned} \tag{15}$$

Before we start looking for the solutions of (15) some comments are necessary. The complexity of the problem is due to the dependence of the interaction strength on the total momentum of the magnons, which is a constant of the motion. Asymptotically, the scattering states can be classified in two classes: (i) a state describing the motion of all free spin waves and (ii) a state describing the motion of a bound pair and a free spin wave. A bound state is defined as a state with energy less than the energies of scattering states. Due to the attractive nature of the nearest-neighbour (NN) interaction, bound states will make the dominant contribution to the amplitude of the component in which all spin reversals lie close to each other. But the next-nearest-neighbour (NNN) interaction partially counterbalances the attractive nature of the NN interaction and hence weakens these bound states [5]. Here, the existence of these bound states is studied as a function of the relative strength parameter α.

Now rewrite equation (15) as

$$\omega U(j,k,l) = \left[H_0 + V_j + V_k + V_l\right] U(j,k,l) \tag{16}$$

where the operators H_0 and V are given by

$$H_0U(j,k,l) = 2S\sum_{CP,i} J(l,i)\big[U(j,k,l) - U(j,k,i)\big] \tag{17}$$

$$V_lU(j,k,l) = J(k,j)\big[U(j,j,l) + U(k,k,l) - 2U(j,k,l)\big]. \tag{18}$$

Here the V_l represent the effect of the pairwise interaction. Define a new function U_l by

$$U_l(j,k,l) = (\omega - H_0)^{-1}V_lU(j,k,l). \tag{19}$$

These new functions are not invariant under permutations of the arguments, but transform as

$$U_l(j,k,l) = U_k(l,j,k) \qquad U_l(j,k,l) = U_l(k,l,j). \tag{20}$$

Also

$$\begin{aligned} U(j,k,l) &= U_l(l,j,k) + U_j(l,j,k) + U_k(l,j,k) \\ &= U_l(l,j,k) + U_l(j,k,l) + U_l(k,l,j). \end{aligned} \tag{21}$$

Then equation (19) becomes

$$U_l(j,k,l) = (\omega - H_0)^{-1}V_l\big[U_l(l,j,k) + U_l(j,k,l) + U_l(k,l,j)\big]. \tag{22}$$

Now introduce the following coordinate system

$$R = \tfrac{1}{3}(R_j + R_k + R_l) \qquad r_l = R_j - R_k \qquad p_l = R_l - \tfrac{1}{2}(R_j + R_k) \tag{23}$$

and define the Fourier transform as

$$U(R,r_l,p_l) = \frac{1}{N^3}\sum_{K,k,\kappa\in F} \exp[i(KR + kr_l + \kappa p_l)]\tilde{U}(K,k,\kappa) \tag{24}$$

where F is the reciprocal lattice. It can be shown that by adding suitable shifts in the basis vectors of F the domain of K, k, and κ can be reorganized such that in one dimension $-\pi \leqslant K, k, \kappa \leqslant \pi$. By obtaining the momentum-space transformations corresponding to coordinates defined in (23), it can be seen that

$$\tilde{U}(K,k,\kappa) = \tilde{U}_l + \tilde{U}_l(K, -\tfrac{1}{2}k + \tfrac{3}{4}\kappa, -k - \tfrac{1}{2}\kappa) + \tilde{U}_l(K, -\tfrac{1}{2}k - \tfrac{3}{4}\kappa, k - \tfrac{1}{2}\kappa). \tag{25}$$

Then, equation (19) finally becomes

$$\begin{aligned} [\omega - E(K,k,\kappa)]\tilde{U}_l(K,k,\kappa) = \frac{2}{N}\sum_{i,k'} J(0,i) \\ \times [2\cos(ki)\cos(\tfrac{1}{3}K - \tfrac{1}{2}\kappa)i - 2\cos(k-k')i][\tilde{U}_l(K,k,\kappa) \\ + \tilde{U}_l(K, -\tfrac{1}{2}k + \tfrac{3}{4}\kappa, -k - \tfrac{1}{2}\kappa) + \tilde{U}_l(K, -\tfrac{1}{2}k - \tfrac{3}{4}\kappa, k - \tfrac{1}{2}\kappa)] \end{aligned} \tag{26}$$

where

$$E(K,k,\kappa) = 4S\sum_i J(0,i)\left[3-\cos(\tfrac{1}{3}K+\kappa)i-2\cos(ki)\cos(\tfrac{1}{3}K-\tfrac{1}{2}\kappa)i\right]. \quad (27)$$

This equation can be further simplified by using the fact that U_l is invariant under interchange of coordinates j and k. Hence

$$\tilde{U}(K,k,\kappa) = \tilde{U}(K,-k,\kappa)$$

Equation (26) reduces to

$$[\omega - E(K,k,\kappa)]\tilde{U}(K,k,\kappa) = \sum_i J(0,i)$$
$$\times\left\{\frac{2}{N}\sum_{k'}[\cos(ki)\cos(\tfrac{1}{3}K-\tfrac{1}{2}\kappa)i-2\cos(k'i)]\right.$$
$$\left.\times\left[\tilde{U}(K,k,\kappa)+2\tilde{U}(K,-\frac{1}{2}k+\tfrac{3}{4}\kappa,-k-\tfrac{1}{2}\kappa)\right]\right\}. \quad (28)$$

For the case $S = 1$, there is a non-physical solution, which has all three spin reversals on the same site. The energy of this state is $6SJ(1+\alpha)$, which is in the continuum.

4. Solution in one dimension

Equation (28) is quite involved and had to be solved numerically. Let us define a new set of functions f_i as

$$f_i(\kappa) = (4/N)\sum_{k'}[\cos(ki)\cos(\tfrac{1}{3}K-\tfrac{1}{2}\kappa)i-\cos(k'i)]$$
$$\times\left[\tilde{U}(K,k,\kappa)+2\tilde{U}(K,-\frac{1}{2}k+\tfrac{3}{4}\kappa,-k-\tfrac{1}{2}\kappa)\right] \quad (29)$$

by means of which equation (28) becomes

$$\tilde{U}(K,k,\kappa) = \sum_i \frac{J(0,i)f_i(\kappa)}{\omega - E(K,k,\kappa)}. \quad (30)$$

With a little effort, by rearranging the domain of k', we get the final equation for f_i

$$f_i(\kappa) = (4/2\pi)\sum_{i'} J(0,i')\left\{\int dk' \frac{\cos(ki)[\cos(\tfrac{1}{3}K-\tfrac{1}{2}\kappa)i-\cos(k'i)]f_{i'}(\kappa)}{\omega - E(K,k',\kappa)}\right.$$
$$\left.+2\int dk' \frac{\cos(ki)[\cos(\tfrac{1}{3}K-\tfrac{1}{2}\kappa)i-\cos(k'+\tfrac{1}{2}\kappa)i]f_{i'}(k')}{\omega - E(K,\tfrac{1}{2}k'+\kappa,\kappa)}\right\}. \quad (31)$$

These integral equations are solved numerically. This set of homogeneous equations for f_i has a nontrivial solution only when the determinant of the coefficients of f_i is zero. To determine the boundary of the scattering region for momentum K, the

energy E_{K_b} of a bound pair with momentum K_b was calculated [5]. If E_{K_f} is the energy of a free magnon with momentum K_f, then the minimum of $E_{K_b} + E_{K_f}$, such that $K_b + K_f = K$, would be the required boundary. The roots of the determinantal equation which lie below this region were determined numerically for different values of K between 0 and π and for values of α up to 1. The solutions reduce to the correct values for $\alpha = 0$ in agreement with Millet and Kaplan [12].

At $\alpha = 0$, the bound states were found for all K, and are strongest for $K = \pi$. A second set of bound states is found, whose energies lie just above the first set. These correspond to the two types of bound states mentioned earlier. However, in this case determining the structure of these states is not easy. For $\alpha > 0$ and $K = \pi$ the bound-state energy rises towards the scattering region with α and finally merges into the scattering region. Figure 1 shows the lowest bound-state energy (dashed line) for different values of α. The boundary of the countinuum is shown by solid lines. The bound states disappear for $K < \pi$ also, but at higher values of α. Figure 2 shows the phase diagram plotted for K versus α. The bound states do not exist in the shaded region.

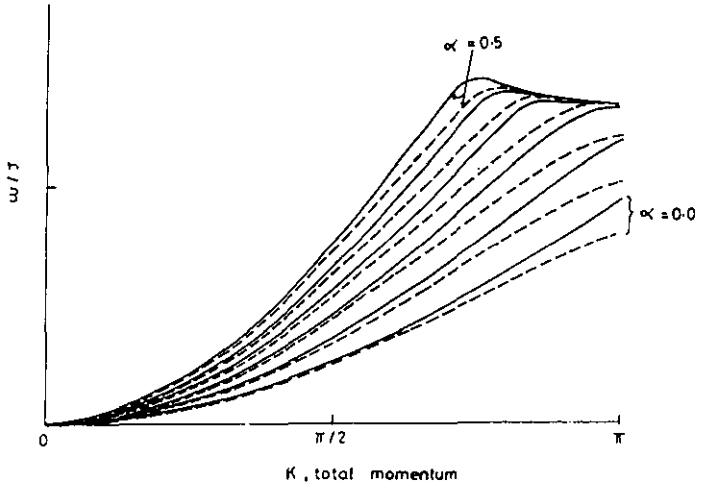

Figure 1. Energies of the lowest bound states for various values of α. Solid lines show the lower boundary of the scattering region. The lowest bound states are shown by dashed lines.

5. Short-chain calculation

The exact diagonalization of the Hamiltonian matrix was done for short chains consisting of up to 40 particles. For closed chains, using C_N invariance of the Hamiltonian, the sizes of the matrices can be reduced considerably. Let the N-particle spin state be written as $|m_1, m_2, \ldots, m_N\rangle$ and

$$S_z |m_1, m_2, \ldots, m_N\rangle = \sum_{j=1}^{N} s_z(j) |m_1, m_2, \ldots, m_N\rangle = \Big(\sum_{j=1}^{N} m_j\Big) |m_1, m_2, \ldots, m_N\rangle.$$

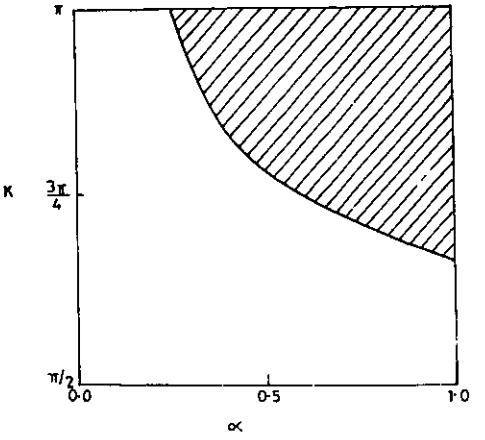

Figure 2. Phase diagram on the K versus α plane. Bound states disappear in shaded region.

Let

$$V = \text{span}\left\{|m_1, m_2, \ldots, m_N\rangle \middle| \left(N - \sum_{j=1}^{N} m_j\right) = 3\right\}$$

Let σ be a 'rotation' operator on V such that

$$\sigma\,|m_1, m_2, \ldots, m_N\rangle = |m_2, m_3, \ldots, m_1\rangle.$$

The group generated by σ is isomorphic to C_N. Then V can be decomposed into

$$V = \bigoplus_{K=0}^{N-1} V_K$$

where V_K contains all invariant subspaces of V equivalent to some irreducible representation of C_N labelled by K. Since $[H, \sigma] = 0$, V_K is invariant under H also. This subspace can be obtained by operating on V with a projection operator

$$P_K = \sum_{i=0}^{N-1} (\epsilon_K \sigma)^i$$

where $\epsilon_K = \exp(\mathrm{i}2\pi K/N)$.

The variable K corresponds to the total momentum of the three magnons. The dimension of V_0 for $N = 40$, is 286 whereas the dimension of V is 11440. Using the above procedure the Hamiltonian matrix was set up for given values of the total momentum K and relative strength parameter α. The matrix was diagonalized to obtain the lowest few eigenenergies and corresponding eigenfunctions.

It was found that the finite-chain calculations for $N \geqslant 30$ agree with the numerical solutions of integral equation to an accuracy of three decimal places. The advantage of the short-chain calculation over the infinite-chain calculation is that by computing

Table 1. Energies of the lowest state and the next lowest state for different values of α.

K	$\alpha = 0.0$		$\alpha = 0.1$		$\alpha = 0.3$		$\alpha = 0.3$		$\alpha = 0.4$		$\alpha = 0.5$	
	A	B	A	B	A	B	A	B	A	B	A	B
0	−0.000	0.050	0.000	0.071	0.000	0.091	−0.000	0.111	−0.000	0.131	−0.000	0.151
$\pi/10$	0.049	0.098	0.068	0.136	0.087	0.174	0.107	0.212	0.126	0.251	0.145	0.289
$2\pi/10$	0.141	0.193	0.197	0.268	0.252	0.343	0.308	0.419	0.363	0.494	0.419	0.569
$3\pi/10$	0.285	0.326	0.396	0.451	0.507	0.576	0.619	0.701	0.730	0.826	0.841	0.950
$4\pi/10$	0.507	0.556	0.700	0.763	0.893	0.970	1.086	1.177	1.278	1.384	1.471	1.591
$5\pi/10$	0.767	0.824	1.052	1.126	1.336	1.426	1.619	1.727	1.902	2.027	2.185	2.327
$6\pi/10$	1.070	1.129	1.453	1.533	1.834	1.938	2.213	2.341	2.591	2.744	2.968	3.147
$7\pi/10$	1.403	1.522	1.882	2.042	2.355	2.553	2.824	3.060	3.289	3.564	3.749	4.065
$8\pi/10$	1.753	1.920	2.316	2.546	2.868	3.165	3.407	3.749	3.928	4.160	4.223	4.257
$9\pi/10$	2.105	2.369	2.733	3.074	3.335	3.714	3.892	4.017	4.055	4.072	4.093	4.093
π	2.382	2.536	3.026	3.254	3.619	3.920	4.000	4.039	4.000	4.067	4.000	4.089

the amplitudes of various components of the wavevector, one can easily identify the structure of the bound states. The lowest bound states have a dominant amplitude corresponding to the basis state in which the three spin reversals lie on three neighbouring sites. A second set of bound states which appear just above these has two spin reversals on one site and a single reversal on a neighbouring site. The energies of these states are given in table 1. For each value of α, column A lists the lowest bound-state energy and column B gives the next lowest states. For $\alpha = 0$, the values reported by Millet and Kaplan as the energy of three bound states are the energies of a bound pair and a free magnon state. The three bound states lie below these values. For $K = \pi$, the eigenvalues of the bound states shift towards the continuum as α increases. For $K < \pi$, the merging occurs at higher values of α.

6. Conclusions

In this report we have investigated the bound-state complexes of three magnons in an $S = 1$ linear chain, which is described by nearest-neighbour (NN) and next-nearest-neighbour (NNN) interactions. The problem was attempted through two methods: (i) by obtaining and numerically solving an integral equation and (ii) by directly diagonalizing finite chains. The results of the two methods agree reasonably well. The integral-equation approach is a straightforward generalization of the treatment by Millet and Kaplan and the results reduce to theirs in the limit $\alpha = 0$.

It was found that bound states vanish as the strength of the NNN interaction increases. This behaviour is the same as for $S = \frac{1}{2}$, the two-magnon case discussed by Majumdar. A new feature in the $S = 1$ case is the existence of two types of bound states. The bound state in which three magnons are on three neighbouring sites has lower energy than the one in which a pair of magnons is on one site and a single magnon on a neighbouring site.

References

[1] Terrance J B and Tinkham T 1969 *Phys. Rev.* **187** 587
[2] Hanus J 1962 *Q. Prog. Rep. Solid State Mol. Theory Group* **43** 96; **44** 38; **46** 137
[3] Fukuda N and Wortis M 1963 *J. Phys. Chem. Solids* **24** 1675
[4] Wortis M 1963 *Phys. Rev.* **132** 85
[5] Majumdar C K 1969 *J. Math. Phys.* **10** 177
[6] Ghosh D K and Mukhopadhyay G 1970 *J. Phys. C: Solid State Phys.* **3** 323
[7] Bethe H K 1931 *Z. Physik* **71** 205
[8] Majumdar C K 1970 *Phys. Rev.* B **1** 287
[9] Faddeev L 1961 *Zh. Eksp. Teor. Fiz.* **39** 1459 (Engl. Transl. *Sov. Phys.–JETP* **12** 1014)
[10] Dyson F J 1956 *Phys. Rev.* **102** 1217
[11] van Himbergen J E 1977 *Physica* A **86** 93
[12] Millet P J and Kaplan H 1973 *Phys. Rev.* B **10** 3923