Spin complexes in a bounded chain

I. G. Gochev

Institute of Solid State Physics, Bulgarian Academy of Sciences, Sofia
(Submitted June 12, 1977)
Pis'ma Zh. Eksp. Teor. Fiz. **26**, No. 3, 136–138 (5 August 1977)

The energy and the wave function are determined for a complex consisting of an arbitrary number of flipped spins and localized near the boundary of a one-dimensional chain.

PACS numbers: 75.10.Hk, 75.30.Ds

It is known that surface spin waves can propagate in a ferromagnet that has a boundary. The bound states of two surface waves were considered in[1] by a variational method. In the one-dimensional case, the analog of such states are spin complexes localized near the boundary of a chain. In the present paper we

 0021-3640/77/2603-0127$00.60

obtain the energy and the wave function of a complex consisting of an arbitrary number of flipped spins and localized near the boundary of a one-dimensional chain. In an infinite chain or in a chain with periodic boundary conditions, the spin complexes (henceforth called volume complexes) were obtained in[2-4].

We write down the Hamiltonian of the ferromagnetic chain in the form

$$H = -J\sum_{l=1}^{N-1}\left[\frac{1}{g}\left(S_l^x S_{l+1}^x + S_l^y S_{l+1}^y\right) + S_l^z S_{l+1}^z\right], \tag{1}$$

where $J>0$, $s=\frac{1}{2}$ and $g\geq 1$. The vector of a state with n flipped spins of the system (1) is represented in the form

$$|\psi_n\rangle = \sum_{m_1, m_2 \ldots m_n} B_{m_1 m_2 \ldots m_n} S_{m_1}^- S_{m_2}^- \ldots S_{m_n}^- |0\rangle ,$$

with $S_m^- \equiv S_m^x - iS_m^y$ and $m_1 < m_2 < \cdots < m_n$. For the amplitudes $B_{m_1 m_2 \ldots m_n}$ we can obtain from the Schrödinger equation a system of equations in the form

$$\left(\varepsilon_n - n + p + \frac{1}{2}\delta_{m_1,1}\right) B_{m_1 m_2 \ldots m_n} + \frac{1}{2g}\sum_{j=1}^{n}{}' \left(B_{m_1 \ldots m_j - 1 \ldots m_n} + B_{m_1 \ldots m_j + 1 \ldots m_n}\right) = 0. \tag{2}$$

Here and below we measure the energy in units of J, $\varepsilon_n = E_n - E_0$, $E_0 = -(N-1)/4$ is the energy of the ground state, p is the number of pairs m_j and m_{j+1} among the indices of the amplitude $B_{m_1 m_2 \ldots m_n}$, such that $m_j = m_{j+1} - 1$. In the sum over j we have left out all the amplitudes with pairs of coinciding indices or with $m_1 = 0$ (see also[4]). Since we are interested in states localized near the boundary, Eqs. (2) take into account the influence of only one end of the chain. Equations (2) differ from the equations for the amplitudes in an infinite chain[4] in the presence of terms with $\delta_{m_1,1}$.

We seek a solution of Eqs. (2) in the form

$$B_{m_1 m_2 \ldots m_n} = A r^{m_1 + m_2 + \ldots + m_n} \prod_{\nu=1}^{n-1} r_\nu^{m_{\nu+1} - m_\nu}, \tag{3}$$

where A is the normalization factor, and r and r_ν are the unknowns.

Substituting (3) in (2) we obtain the following $n+1$ independing equations ($r_0 \equiv r_n \equiv 1$):

$$\varepsilon_n = n - \frac{1}{2g}\sum_{j=0}^{n-1}\left(\frac{r_{j+1}}{r r_j} + \frac{r r_j}{r_{j+1}}\right), \tag{4a}$$

$$2g r_\nu = r r_{\nu-1} + \frac{1}{r} r_{\nu+1}, \quad \nu = 1, 2, \ldots, n-1, \tag{4b}$$

$$g r = r_1. \tag{4c}$$

There is a close similarity between relations (3), (4a), and (4b), on the one hand, and the relations for the case of complexes in an infinite chain,[4] namely, the equations written out here are obtained from the corresponding

ones in[4] by replacing $\exp(ik/n)$ by r. Using the solution of[4] for volume complexes, we obtain the solution of Eqs. (4a)—(4c):

$$r = (\operatorname{ch} n\sigma)^{-1/n}, \quad r_\nu = \operatorname{ch}\nu\sigma(\operatorname{ch} n\sigma)^{-\nu/n},$$
$$\varepsilon_n = \frac{1}{2}\operatorname{th}\sigma \operatorname{th} n\sigma, \tag{5}$$

where $\sigma = \ln(g + \sqrt{g^2-1})$.

It can be verified that at $g>1$ we have $0 \le r < 1, 0 < r_\nu < 1$, i.e., in the state with the wave function (3) the flipped spins are bound into a complex localized near the boundary. In an isotropic chain ($g=1$) the complex does not exist. An analysis of the solution (5) shows the following: 1) the bonds between the spins and the complex are the strongest near the boundary and weaken with increasing distance from the boundary; 2) the energy ε_n is less than the energy of a volume complex having the same number n of flipped spins; 3) $\varepsilon_n < \varepsilon_{n-1} + 1 - 1/g$ ($1 - 1/g$ is the minimal energy of the volume magnon); 4) $\varepsilon_n > \varepsilon_{n-1}$ (at large k the inverse inequality is satisfied for volume complexes); 5) at $n \gg 1$ we have $\varepsilon_n = (\frac{1}{2})\tanh\sigma$ (for volume complexes this limit is equal to $\tanh\sigma$). Thus, surface complexes lie in the energy interval $[(\frac{1}{2})\tanh^2\sigma, (\frac{1}{2})\tanh\sigma]$. We note that volume spin complexes with large n have been recently observed in a three-dimensional ferromagnet[5]; 6) in a strongly anisotropic chain ($g \gg 1$) we have at $n \ge 2$

$$\varepsilon_n = \frac{1}{2}\left(1 - \frac{1}{2g^2}\right), \tag{6}$$

in the Ising model we have $g \to \infty$ and $\varepsilon_n = \frac{1}{2}$.

In the case of a finite chain, localized n-particle states of another type are possible, wherein a complex of $n-q$ flipped spins is captured on one end of the chain, and a complex of q spins is captured on the other (of course, N is assumed to be much larger than the characteristic dimensions of the complexes). We can prove the inequality $\varepsilon_n < \varepsilon_{n-q} + \varepsilon_q$, i.e., the surface spin complex has the lowest energy from among all the n-particle states of the system (1). At $n = 2$, the solution of our problem was obtained earlier in[1].

In the case of a chain with periodic boundary conditions, the uniqueness of the spin complex obtained in[2-4] follows from the total analysis of Bethe[2] and Ohrbach.[7] Although no analogous complete investigation has been made in the case of an open chain, the fact that in the (one-dimensional) Ising model there exists one surface complex suggests that the complex obtained here is the only surface complex in the model (1) at arbitrary $q>1$.

In a one-dimensional $CoCl_2 \cdot 2H_2O$ chain, volume spin complexes were observed in experiment up to $n = 14$.[6] As already discussed in[1], this substance is apparently suitable for the excitation of surface complexes. Since $q \gg 1$ for $CoCl_2 \cdot 2H_2O$, the energy of the surface complexes is described by formula (6).

[1]S.T. Chiu-Tsao, Phys. Rev. B 11, 4525 (1975).
[2]H. Bethe, Z. Phys. 71, 205 (1931).

[3]A. A. Ovchinnikov, Pis'ma Zh. Eksp. Teor. Fiz. 5, 48 (1967) [JETP Lett. 5, 38 (1967)].
[4]I. G. Gochev, Zh. Eksp. Teor. Fiz. 61, 1674 (1971) [Sov. Phys. JETP 34, 892 (1972)].
[5]B. A. Ivanov and A. M. Kosevich, Pis'ma Zh. Eksp. Teor. Fiz. 24, 495 (1976) [JETP Lett. 24, 454 (1976)].
[6]J. Torrance and M. Tinkham, Phys. Rev. 187, 587 (1969); D. Nicoli and M. Tinkham, Phys. Rev. B 9, 3126 (1974).
[7]R. Orbach, Phys. Rev. 112, 309 (1968).