Ground state and excitations of a spin chain with orbital degeneracy

You-Quan Li

Department of Physics, University of Cincinnati, Cincinnati Ohio 45221 and Zhejiang Institute of Modern Physics, Zhejiang University, Hangzhou 310027, China

Michael Ma

Department of Physics, University of Cincinnati, Cincinnati, Ohio 45221

Da-Ning Shi

Department of Physics, University of Cincinnati, Cincinnati, Ohio 45221 and College of Science, Nanjing University of Aeronautics and Astronautics, Nanjing, China

Fu-Chun Zhang

Department of Physics, University of Cincinnati, Cincinnati, Ohio 45221

(Received 3 May 1999)

The one-dimensional Heisenberg model in the presence of orbital degeneracy is studied at the SU(4) symmetric point by means of Bethe ansatz. Following Sutherland's previous work on an equivalent model, we discuss the ground state and the low-lying excitations more extensively in connection to the spin systems with orbital degeneracy. We show explicitly that the ground state is a SU(4) singlet. We study the degeneracies of the elementary excitations and the spectra of the generalized magnons consisting of these excitations. We also discuss the complex 2-strings in the context of the Bethe ansatz solutions. [S0163-1829(99)00238-6]

I. INTRODUCTION

There has been much interest recently in spin Hamiltonians with orbital degeneracy. The orbital degree of freedom may be relevant to many transitional-metal oxides.^{1–11} Examples of such systems in one dimension include quasi-onedimensional tetrahis-dimethylamino-ethylene (TDAE)-C₆₀ (Ref. 12) and artificial quantum dot arrays.¹³ Recently, we discussed these systems¹⁴ within the framework of a *SU*(4) theory. A quantum disordered ground state in two dimensions was proposed to be relevant to the experimentally observed unusual magnetic properties in LiNiO₂. There have also been numerical studies of the one-dimensional models for these systems.^{15,16}

In the present paper, we use the Bethe ansatz method to study the SU(4) symmetric Heisenberg spin chain with twofold orbital degeneracy. This model is equivalent to the model studied by Pokrovskii and Uimin,¹⁷ and to one of a class of models that has been solved by Sutherland.¹⁸ Expanding on Sutherland's work, we study the ground state and low-lying excitations more extensively by considering holes and 2-strings in the thermodynamics limit, and in connection to the spin systems with orbital degeneracy. We show explicitly that the ground state is a SU(4) singlet, consistent with the generalized Lieb-Mattis theorem of Affleck and Lieb.²² We discuss the degeneracies of the elementary excitations and the spectra of the generalized magnons resulting from such excitations. We also discuss the complex 2-strings in the context of the Bethe ansatz solutions. The paper is organized as follows. In Sec. II, we introduce the model and discuss its symmetry. In Sec. III, we present the Bethe ansatz solution following Sutherland's approach. We discuss the ground state in Sec. IV, and the elementary excitations and

the generalized magnon modes in Sec. V. A brief summary is given in Sec. VI.

II. SYMMETRY CONSIDERATION

We consider the spin chain of N sites with twofold orbital degeneracy and with periodic boundary condition⁶

$$\mathcal{H} = \sum_{j=1}^{N} J \left[\left(2\vec{T}_{j} \cdot \vec{T}_{j+1} + \frac{1}{2} \right) \left(2\vec{S}_{j} \cdot \vec{S}_{j+1} + \frac{1}{2} \right) - 1 \right], \quad (1)$$

where \tilde{S}_j and \tilde{T}_j are the spin and orbital operators respectively on the *j*th site, and are each generators of a SU(2) Lie algebra. Clearly, in addition to the permutation symmetry (*H* is invariant under the transformation $j \rightarrow j + 1$ for all *j*'s), the system has an explicit $SU(2) \otimes SU(2)$ global symmetry and a bisymmetry $\tilde{S}_j \leftrightarrow \tilde{T}_j$. Actually the Hamiltonian (1) is invariant under a global SU(4) transformation, which is generated by $S^{\alpha} = \sum_j S_j^{\alpha}$, $T^{\alpha} = \sum_j T_j^{\alpha}$, and $Y^{\alpha\beta} = \sum_j T_j^{\alpha} \otimes S_j^{\beta}$ ($\alpha, \beta = 1, 2, 3$). These operators satisfy the following commutation relations:

$$[S^{\alpha}, S^{\beta}] = i \epsilon^{\alpha \beta \gamma} S^{\gamma}, \quad [S^{\alpha}, T^{\beta}] = 0,$$

$$[T^{\alpha}, T^{\beta}] = i \epsilon^{\alpha \beta \gamma} T^{\gamma}, \quad [T^{\alpha}, Y^{\beta \delta}] = i \epsilon^{\alpha \beta \gamma} Y^{\gamma \delta},$$

$$[S^{\alpha}, Y^{\delta \beta}] = i \epsilon^{\alpha \beta \gamma} Y^{\delta \gamma},$$

$$[Y^{\alpha \mu}, Y^{\beta \nu}] = i \epsilon^{\alpha \beta \gamma} \delta^{\mu \nu} S^{\gamma} + i \epsilon^{\mu \nu \rho} \delta^{\alpha \beta} T^{\rho}.$$
 (2)

Such a symmetry was noticed by Wigner in the study of nuclei a long time ago.¹⁹ Since the group SU(4) is of rank 3, there are three conserved quantum numbers in general. It is useful to write the above commutation relations in terms of

12 781

Chevalley basis, i.e., three generators in the Cartan subalgebra of SU(4) (precisely, the A_3 Lie algebra) $H_n = \sum_{j=1}^{N} H_n(j)$ (n=1, 2, 3) which can be diagonalized simultaneously, and the other 12 generators $E_{\alpha} = \sum_{j=1}^{N} E_{\alpha}(j)$ (α denotes root vectors). The local generators $H_n(j)$ and $E_{\alpha}(j)$ are related to the spin and orbital operators by

$$\begin{split} H_{1}(j) &= (1+2T_{j}^{z})S_{j}^{z}, \quad E_{\alpha_{1}}(j) = \left(\frac{1}{2}+T_{j}^{z}\right)S_{j}^{+}, \\ H_{2}(j) &= (T_{j}^{z}-S_{j}^{z}), \quad E_{\alpha_{2}}(j) = T_{j}^{+}S_{j}^{-}, \\ H_{3}(j) &= (1-2T_{j}^{z})S_{j}^{z}, \quad E_{\alpha_{3}}(j) = \left(\frac{1}{2}-T_{j}^{z}\right)S_{j}^{+}, \\ E_{\alpha_{1}+\alpha_{2}}(j) &= T_{j}^{+}\left(\frac{1}{2}+S_{j}^{z}\right), \\ E_{\alpha_{2}+\alpha_{3}}(j) &= T_{j}^{+}\left(\frac{1}{2}-S_{j}^{z}\right), \\ E_{\alpha_{1}+\alpha_{2}+\alpha_{3}}(j) &= T_{j}^{+}S_{j}^{+}, \end{split}$$
(3)

where α_1 , α_2 , and α_3 denote the simple roots of A_3 Lie algebra.²¹ The generators corresponding to the negative roots are given by $E_{-\alpha}(j) = E_{\alpha}^{\dagger}(j)$. One can verify that these operators satisfy the standard commutation relations of A_3 Lie algebra, and Eq. (1) can be rewritten as

$$\mathcal{H} = \sum_{j} [h(j,j+1) - 3/4],$$
$$h(j,j+1) = \sum_{m,n} g^{mn} H_m(j) H_n(j+1)$$
$$+ \sum_{\alpha \in \Delta} E_\alpha(j) E_{-\alpha}(j+1),$$

where Δ denotes the set of roots of the Lie algebra. We denote the spin components by up (\uparrow) and down (\downarrow), and the orbital components by top and bottom. Then the four possible states on each site are

$$|1\rangle := |^{\uparrow}_{-}\rangle = |1/2, 1/2\rangle,$$

$$|2\rangle := |^{\downarrow}_{-}\rangle = |-1/2, 1/2\rangle,$$

$$|3\rangle := |^{-}_{\uparrow}\rangle = |1/2, -1/2\rangle,$$

$$|4\rangle := |^{-}_{\downarrow}\rangle = |-1/2, -1/2\rangle.$$

The local lowering/raising operators $E_{\pm \alpha_n}(j)$ relate those four states on the *j*th site as follows:

$$E_{-\alpha_n}(j)|n\rangle_j \rightarrow |n+1\rangle_j,$$

$$E_{\alpha_n}(j)|n+1\rangle_j \rightarrow |n\rangle_j, \quad n=1,2,3.$$
(4)

In terms of those operators, a general state can be written as

$$|\psi\rangle = \sum_{\{x_i\}\{y_j\}\{z_k\}} \psi(x;y;z) \prod_{k=1}^{M} E_{-\alpha_3}(z_k)$$
$$\times \prod_{j=1}^{M'} E_{-\alpha_2}(y_j) \prod_{i=1}^{M} E_{-\alpha_1}(x_i)|_{--}^{\uparrow\uparrow} \cdots \stackrel{\uparrow}{-}\rangle, \qquad (5)$$

M''

where $x := (x_1, x_2, \ldots, x_M)$, $y := (y_1, y_2, \ldots, y_M')$, $z := (z_1, z_2, \ldots, z_{M''})$; $1 \le x_1 < x_2 < \ldots < x_M \le N$; $x_1 \le y_1 < y_2 < \ldots < y_{M'} \le x_M$, $y_1 \le z_1 < z_2 < \ldots < z_{M''} \le y_{M'}$; and $\{z_k\} \subset \{y_j\} \subset \{x_i\}$. We may define the weights as the eigenvalues of the global operator H_n , indicated by (H_1, H_2, H_3) . The eigenvalues of the local operators $H_1(j), H_2(j), H_3(j)$ acting on the four local states $|\uparrow\rangle_j$, $|\downarrow\rangle_j$, $|\uparrow\rangle_j$, and $|\downarrow\rangle_j$ are (1,0,0), (-1,1,0), (0,-1,1), and (0,0,-1), respectively. We shall focus on the state with the highest weight. The other states in the same irreducible representation can then be obtained by using the corresponding lowering operators $E_{-\alpha_n}$. In the present model, the irreducible representation of the SU(4) group of a *N*-site system is labeled by

$$(N+M'-2M, M+M''-2M', M'-2M'').$$
 (6)

III. THE BETHE ANSATZ SOLUTION

The permutation and the SU(4) symmetries in the Hamiltonian enable us to seek the eigenstate of both the cyclic permutation operator and the generators of the Cartan subalgebra of A_3 . The invariance of the cyclic permutation imposes a periodic boundary condition on the wave function $\psi(x,y,z)$. The present model is solvable,¹⁸ and the Bethe ansatz equations for the spectra are

$$\left(\frac{\lambda_{j}+i/2}{\lambda_{j}-i/2}\right)^{N} = -\prod_{l=1}^{M} \frac{\lambda_{j}-\lambda_{l}+i}{\lambda_{j}-\lambda_{l}-i} \prod_{\beta=1}^{M'} \frac{\mu_{\beta}-\lambda_{j}+i/2}{\mu_{\beta}-\lambda_{j}-i/2},$$

$$\prod_{l=1}^{M} \frac{\mu_{\gamma}-\lambda_{l}+i/2}{\mu_{\gamma}-\lambda_{l}-i/2} = -\prod_{\beta=1}^{M'} \frac{\mu_{\gamma}-\mu_{\beta}+i}{\mu_{\gamma}-\mu_{\beta}-i} \prod_{b=1}^{M''} \frac{\nu_{b}-\mu_{\gamma}+i/2}{\nu_{b}-\mu_{\gamma}-i/2},$$

$$\prod_{\beta=1}^{M'} \frac{\nu_{c}-\mu_{\beta}+i/2}{\nu_{c}-\mu_{\beta}-i/2} = -\prod_{b=1}^{M''} \frac{\nu_{c}-\nu_{b}+i}{\nu_{c}-\nu_{b}-i},$$

$$(7)$$

where j, l = 1, 2, ..., M; $\beta, \gamma = 1, 2, ..., M'$ and b, c = 1, 2, ..., M''. These are secular equations for the spectra of SU(4) rapidities λ , μ , and ν . The energy spectrum is given by

$$E = -\sum_{l=1}^{M} \frac{J}{(1/2)^2 + \lambda_l^2}.$$
(8)

The momentum defined by the translation of the system along the chain is given by

$$P = \frac{1}{i} \ln \prod_{l=1}^{M} \frac{\lambda_l + i/2}{\lambda_l - i/2} = \sum_{l=1}^{M} \left[\pi - 2 \tan^{-1}(2\lambda_l) \right].$$
(9)

Note that *P* in Eq. (9) is determined up to mod (2π) , and the inverse trigonometric function is defined in the main branch. We have included explicitly the π term in Eq. (9), which is usually neglected in the study of pure spin Heisenberg

models.²⁰ In the SU(4) model, there are three types of elementary excitations as we will discuss below, and it is convenient to include the π term in *P* to study the magnon types of composite excitations. We define the momentum of the elementary excitations as the momentum relative to the ground state.²⁰ By taking the logarithm of Eq. (7), a set of coupled transcendental equations are obtained,

$$\begin{split} \Theta_{1/2}(\lambda_j) &- \frac{1}{N} \sum_{l=1}^M \Theta_1(\lambda_j - \lambda_l) - \frac{1}{N} \sum_{\beta}^{M'} \Theta_{1/2}(\mu_{\beta} - \lambda_j) \\ &= \frac{2\pi}{N} I_j, \end{split}$$

$$\sum_{l=1}^{M} \Theta_{1/2}(\mu_{\gamma} - \lambda_{l}) - \sum_{\beta=1}^{M'} \Theta_{1}(\mu_{\gamma} - \mu_{\beta}) - \sum_{b=1}^{M''} \Theta_{1/2}(\nu_{b} - \mu_{\gamma})$$

= $2 \pi J_{\gamma}$,
$$\sum_{\beta=1}^{M'} \Theta_{1/2}(\nu_{c} - \mu_{\beta}) - \sum_{b=1}^{M''} \Theta_{1}(\nu_{c} - \nu_{b}) = 2 \pi K_{c}, \quad (10)$$

where $\Theta_{\rho}(x) := 2 \tan^{-1}(x/\rho)$. The quantum number I_j is an integer or half integer depending on whether N - M - M' is odd or even, and so is J_{γ} (or K_c) depending on whether M - M' - M'' (or M' - M'') is odd or even. These properties arise from the logarithm function.

Replacing λ_j , μ_{γ} , and ν_c in Eq. (10) by continuous variables λ , μ , and ν but keeping the summation still over the solution set of these roots $\{\lambda_l, \mu_{\beta}, \nu_b\}$, we can consider the quantum numbers I_j , J_{γ} , and K_c as functions $I(\lambda)$, $J(\mu)$, and $K(\nu)$ given by Eq. (10). Take $I(\lambda)$ as an example. When $I(\lambda)$ passes through one of the quantum numbers I_j , the corresponding λ is equal to one of the roots λ_j . Similarly for $J(\mu)$ or $K(\nu)$. However, there may exist some integers or half integers for which the corresponding λ (μ or ν) is not in the set of roots. We shall name such a state as a "hole." In the thermodynamics limit $N \rightarrow \infty$, we may introduce the density of roots and the density of holes (indicated by a subscript h):

$$\sigma(\lambda) + \sigma_h(\lambda) = (1/N) dI(\lambda)/d\lambda,$$

$$\omega(\mu) + \omega_h(\mu) = (1/N) dJ(\mu)/d\mu,$$

$$\tau(\nu) + \tau_h(\nu) = (1/N) dK(\nu)/d\nu.$$

By replacing the summations by integrals,

$$\begin{split} &\lim_{N\to\infty} \frac{1}{N} \sum_{l=1}^{M} f(\lambda_l) = \int_{-B}^{B} d\lambda \,\sigma(\lambda) f(\lambda), \\ &\lim_{N\to\infty} \frac{1}{N} \sum_{\beta=1}^{M'} f(\mu_{\beta}) = \int_{-B'}^{B'} d\mu \,\omega(\mu) f(\mu), \\ &\lim_{N\to\infty} \frac{1}{N} \sum_{b=1}^{M''} f(\nu_b) = \int_{-B''}^{B''} d\nu \tau(\nu) f(\nu), \end{split}$$

 $\sigma(\lambda) + \sigma_{h}(\lambda) = K_{1/2}(\lambda) - \int_{-B}^{B} d\lambda' K_{1}(\lambda - \lambda') \sigma(\lambda')$ $+ \int_{-B'}^{B'} d\mu' K_{1/2}(\lambda - \mu') \omega(\mu'),$ $\omega(\mu) + \omega_{h}(\mu) = \int_{-B}^{B} d\lambda' K_{1/2}(\mu - \lambda') \sigma(\lambda')$ $- \int_{-B'}^{B'} d\mu' K_{1/2}(\mu - \mu') \omega(\mu')$ $+ \int_{-B''}^{B''} d\nu' K_{1/2}(\mu - \nu') \tau(\nu'),$ $\tau(\nu) + \tau_{h}(\nu) = \int_{-B'}^{B'} d\mu' K_{1/2}(\nu - \mu') \omega(\mu')$ $- \int_{-B''}^{B''} d\nu' K_{1}(\nu - \nu') \tau(\nu'),$ (11)

where $K_{\rho}(x) \coloneqq \pi^{-1} \rho / (\rho^2 + x^2)$, and *B*, *B'*, and *B''* in the definite integrals should be determined self-consistently. In the absence of the complex roots, $M/N = \int_{-B}^{B} \sigma(\lambda) d\lambda$, $M'/N = \int_{-B'}^{B'} \omega(\mu) d\mu$, and $M''/N = \int_{-B''}^{B''} \tau(\nu) d\nu$. Once the density σ is solved from Eq. (11), we have the *z* components of the total spin and the total orbital:

$$\frac{S_{tot}^{z}}{N} = \frac{1}{2} + \int_{-B'}^{B'} \omega(\mu) d\mu - \int_{-B}^{B} \sigma(\lambda) d\lambda - \int_{-B''}^{B''} \tau(\nu) d\nu,$$
$$\frac{T_{tot}^{z}}{N} = \frac{1}{2} - \int_{-B'}^{B'} \omega(\mu) d\mu, \qquad (12)$$

the energy

$$E = -2 \pi N J \int_{-B}^{B} K_{1/2}(\lambda) \sigma(\lambda) d\lambda,$$

and the momentum

$$P = -N \int_{-B}^{B} [2 \tan^{-1}(2\lambda) - \pi] \sigma(\lambda) d\lambda.$$

IV. THE GROUND STATE

The ground state is described by the densities $\sigma_0(\lambda)$, $\omega_0(\mu)$, and $\tau_0(\nu)$ with no holes and by $B_0 = B'_0 = B''_0 \rightarrow \infty$. This is true because all the states with holes will have higher energies. In this case, Eq. (11) can be solved. Let

$$\sigma_{0}(\lambda) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{\sigma}_{0}(q) e^{-iq\lambda} dq,$$
$$\omega_{0}(\mu) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{\omega}_{0}(q) e^{-iq\mu} dq,$$
$$\tau_{0}(\nu) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{\tau}_{0}(q) e^{-iq\nu} dq,$$

Eq. (9) becomes the coupled integral equations

then

$$\widetilde{\omega}_{0}(q) = \sinh(3q/2)/\sinh(2q),$$
$$\widetilde{\omega}_{0}(q) = \sinh(q)/\sinh(2q),$$
$$\widetilde{\tau}_{0}(q) = \sinh(q/2)/\sinh(2q).$$

Hence from Eq. (6), the highest weight labeling the ground state is the null vector (0, 0, 0), and so the ground state is a SU(4) singlet. This agrees to the theorem of Affleck and Lieb,²² a generalization of the spin chain problem.^{23,24} In that state, the total orbital, the total spin, and their products are all zero, i.e.,

$$\begin{aligned} T_{tot}^z &= \frac{1}{2} - \int_{-\infty}^{\infty} \omega_0(\mu) d\mu = \frac{1}{2} - \tilde{\omega}_0(0) = 0, \\ S_{tot}^z / N &= \frac{1}{2} + \tilde{\omega}_0(0) - \tilde{\sigma}_0(0) - \tilde{\tau}_0(0) = 0, \\ &\sum_{j=1}^N T_j^z S_j^z = 0. \end{aligned}$$

In deriving this result, Eqs. (3) have been used. The energy and the momentum of the ground state are

$$E_0 = -NJ\left(\frac{3}{2}\ln 2 + \frac{\pi}{4}\right)$$

$$P_0 = \begin{cases} 0 \mod 2\pi & \text{for } N/4 = \text{even} \\ \pi \mod 2\pi, & \text{for } N/4 = \text{odd.} \end{cases}$$
(13)

Equation (13) coincides with the result of Sutherland¹⁸ after correcting for the trivial overall constant shift JN between the two models.

V. LOW-LYING EXCITATIONS

A. Spectra of elementary excitations

The possible elementary excitation modes are obtained by the variation in the sequence of quantum numbers $\{I_j\}, \{J_\gamma\},$ or $\{K_c\}$ from the ground state. We can assume $B = B' = B'' \rightarrow \infty$ for the low-lying excitations. The simple modes will be solved by placing holes in the rapidity configurations. If we let $\sigma(\lambda) = \sigma_0(\lambda) + \sigma_1(\lambda)/N$, $\omega(\mu) = \omega_0(\mu) + \omega_1(\mu)/N$ and $\tau(\nu) = \tau_0(\nu) + \tau_1(\nu)/N$, then the excitation energy and momentum,

$$\Delta E = -2\pi J \int_{-\infty}^{\infty} K_{1/2}(\lambda) \sigma_1(\lambda) d\lambda,$$

$$\Delta P = -\int_{-\infty}^{\infty} [2\tan^{-1}(2\lambda) - \pi] \sigma_1(\lambda) d\lambda, \qquad (14)$$

and $\Delta M = \int \sigma_1(\lambda) d\lambda$, $\Delta M' = \int \omega_1(\mu) d\mu$, and $\Delta M'' = \int \tau_1(\nu) d\nu$. After solving the integral Eqs. (11) with $\sigma_h(\lambda) = \delta(\lambda - \overline{\lambda})/N$, $\omega_h(\mu) = \delta(\mu - \overline{\mu})/N$ or $\tau_h(\nu) = \delta(\nu - \overline{\nu})/N$, respectively, one finds that there are three types of elementary excitation modes. A hole in the λ configuration, μ configuration, or ν configuration (λ hole, μ hole, and ν hole, respectively, hereafter) creates a SU(4) multiplet labeled by the highest weight (1, 0, 0), (0, 1, 0), or (0, 0, 1),



FIG. 1. The spectra of the three types of quasiparticles.

respectively. The μ hole has a six-dimensional representation, the λ and ν holes have four-dimensional representation. We call these excitations the SU(4) flavorons. The energies of these elementary excitations are

$$\varepsilon_{\sigma}(\bar{\lambda}) = \frac{J\pi/2}{\sqrt{2}\cosh(\bar{\lambda}\pi/2) - 1},$$

$$\varepsilon_{\omega}(\bar{\mu}) = \frac{J\pi/2}{\cosh(\pi\bar{\mu}/2)},$$

$$\varepsilon_{\tau}(\bar{\nu}) = \frac{J\pi/2}{\sqrt{2}\cosh(\bar{\nu}\pi/2) + 1},$$
(15)

where $\overline{\lambda}$, $\overline{\mu}$, and $\overline{\nu}$ stand for the positions of holes in the corresponding rapidity configurations. These excitation energies vanish when the positions of holes go to infinity in the thermodynamic limit. Therefore they are gapless modes. The momenta of the excitations are given by

$$p_{\sigma}(\bar{\lambda}) = 2 \tan^{-1} [(\sqrt{2} + 1) \tanh(\bar{\lambda} \pi/4)] - 3\pi/4,$$
$$p_{\omega}(\bar{\mu}) = 2 \tan^{-1} [\tanh(\bar{\mu} \pi/4)] - \pi/2,$$
$$p_{\tau}(\bar{\nu}) = 2 \tan^{-1} [(\sqrt{2} - 1) \tanh(\bar{\nu} \pi/4)] - \pi/4.$$
(16)

Eliminating the rapidities in Eqs. (15) and (16), we have

$$\varepsilon_{\sigma}(p_{\sigma}) = \frac{J\pi}{2} [\sqrt{2} \cos(p_{\sigma} + 3\pi/4) + 1],$$

$$\varepsilon_{\omega}(p_{\omega}) = \frac{J\pi}{2} \cos(p_{\omega} + \pi/2),$$

$$\varepsilon_{\tau}(p_{\tau}) = \frac{J\pi}{2} [\sqrt{2} \cos(p_{\tau} + \pi/4) - 1],$$
(17)

where $p_{\sigma} \in [-3\pi/2,0], p_{\omega} \in [-\pi,0], p_{\tau} \in [-\pi/2,0].$

We are now in the position to relate the elementary excitations to the spin and orbital in the original model, Eq. (1). The quadruplets (1, 0, 0) or (0, 0, 1) are flavorons carrying both spin 1/2 and orbital 1/2 with energies ϵ_{σ} or ϵ_{τ} , the hexaplet (0, 1, 0) describes flavorons carrying either spin 1 or orbital 1 with energy ϵ_{ω} . The spectra of these three types of excitations are plotted in Fig. 1. In comparison to Sutherland's results, Eq. (17) differs only in that each mode is shifted by a different constant in momentum arising from the



FIG. 2. The dispersions for various types of the generalized magnons. E and P stand for the the corresponding ΔE and ΔP in Sec. V C.

 π term in Eq. (9). It seems more convenient to use the present version, Eq. (17), to study the spectra of the magnon-type excitations in Sec. V C.

B. The complex roots

Because of the existance of the complex roots²⁵ in the solution set of the Bethe ansatz Eqs. (7), we must consider their contributions, particularly from the 2-strings. In this case we need to rederive the integral Eqs. (11). We obtain the same equation formally but now the inhomogeneous terms $\sigma_h(\lambda)$, $\omega_h(\mu)$, and $\tau_h(\nu)$ include also the contributions from the complex roots. A 2-string in the λ configuration, $\lambda_{\pm} = \lambda_0 \pm i/2$, introduces additional terms in Eq. (11). As a result, we have

$$\sigma_h(\lambda) = [K_{3/2}(\lambda - \lambda_0) + K_{1/2}(\lambda - \lambda_0)]/N,$$
$$\omega_h(\mu) = -K_1(\mu - \lambda_0)/N,$$
$$\tau_h(\nu) = 0. \tag{18}$$

The energy is given by

$$\Delta E = -2 \pi J \int_{-\infty}^{\infty} K_{1/2}(\lambda) \sigma_1(\lambda) d\lambda - 2 \pi J [K_{1/2}(\lambda_0 + i/2) + K_{1/2}(\lambda_0 - i/2)], \qquad (19)$$

and the integral equation leads to

$$\widetilde{\sigma}_1(q) = -\exp(iq\lambda_0 - |q|/2).$$

Our calculation shows a complete cancellation in Eq. (19). Therefore a 2-string in the λ configuration does not change the energy. We also find $M = N \int \sigma(\lambda) d\lambda + 2$, where $\sigma(\lambda)$ is the density of the real roots.

Similar results are found for the 2-strings in the ν and μ configurations. The equations for a ν configuration are given by

$$\sigma_h(\lambda) = 0,$$

$$\omega_h(\mu) = -K_1(\mu - \nu_0)/N,$$

$$\nu) = [K_{3/2}(\nu - \nu_0) + K_{1/2}(\nu - \nu_0)]/N,$$

and $M'' = N \int \tau(\nu) d\nu + 2$. By solving $\sigma_1(\lambda) = 0$, we obtain

 $\tau_h($

$$\Delta E = -2 \pi J \int K_{1/2} \sigma_1(\lambda) d\lambda = 0.$$

And the equations for a 2-string in the μ configuration are given by

$$\sigma_h(\lambda) = -K_1(\lambda - \mu_0)/N,$$

$$\omega_h(\mu) = [K_{1/2}(\mu - \mu_0) + K_{3/2}(\mu - \mu_0)]/N,$$

$$\tau_h(\nu) = -K_1(\nu - \mu_0)/N,$$

and $M' = N \int \omega(\mu) d\mu + 2$, we obtain $\sigma_1(\lambda) = 0$ and hence $\Delta E = 0$. Although these three types of the 2-strings do not contribute to the energy, they do contribute to the quantum numbers of spin and orbital, and to the highest weight of the SU(4) representations.

C. Generalized magnon-type excitations

The flavorons discussed in the previous subsection are elementary excitations of the system. These flavorons may combine to form composite excitations similar to the magnon excitations in the one-dimensional spin chain,²⁶ which are of interest to experiments and numerical simulations. In such a construction, the structure of the decomposition of the

direct product of the SU(4) fundamental representation must be taken into account. Let us consider N=4n, the decomposition brings about a direct sum of a series of irreducible representations, i.e., (0,0,0), (1,0,1), (0,2,0), (2,1,0), (4,0,0), etc. The composite excitation states include both the singlet (0,0,0) and the multiplets of 15-fold (1,0,1), of 20-fold (0,2,0), and of 45-fold (2,1,0), or of 35-fold (4,0,0), etc. Those multifold excitations are the generalization of magnon excitations to the spin systems with orbital degeneracy. One λ hole and one ν hole together create a 15-fold multiplet with excitation energy and momentum,

$$\Delta E_{(15)} = \varepsilon_{\sigma}(\bar{\lambda}) + \varepsilon_{\tau}(\bar{\nu}),$$

$$\Delta P_{(15)} = p_{\sigma}(\bar{\lambda}) + p_{\tau}(\bar{\nu}),$$

which is a pair of flavorons of σ type and τ type. Two μ holes create a 20-fold multiplet with

$$\Delta E_{(20)} = \varepsilon_{\omega}(\bar{\mu}_1) + \varepsilon_{\omega}(\bar{\mu}_2),$$

$$\Delta P_{(20)} = p_{\omega}(\bar{\mu}_1) + p_{\omega}(\bar{\mu}_2).$$

The 45-fold multiplet is a three-hole state created by two λ holes and one μ hole, for which the excitation energy and momentum are

$$\Delta E_{(45)} = \varepsilon_{\sigma}(\bar{\lambda}_{1}) + \varepsilon_{\sigma}(\bar{\lambda}_{2}) + \varepsilon_{\omega}(\bar{\mu}),$$

$$\Delta P_{(45)} = p_{\sigma}(\bar{\lambda}_{1}) + p_{\sigma}(\bar{\lambda}_{2}) + p_{\omega}(\bar{\mu}).$$

Four λ holes create a 35-fold multiplet with

$$\Delta E_{(35)} = \sum_{j=1}^{4} \varepsilon_{\sigma}(\bar{\lambda}_{j}),$$
$$\Delta P_{(35)} = \sum_{j=1}^{4} p_{\sigma}(\bar{\lambda}_{j}).$$

The singlet excitation is obtained by placing a λ hole, a ν hole, and three 2-strings in λ , μ , and ν configurations, respectively. The singlet is degenerate with the 15-fold multiplet in energy, i.e.,

$$\Delta E_{(1)} = \varepsilon_{\sigma}(\overline{\lambda}) + \varepsilon_{\tau}(\overline{\nu}).$$

In the above equations, $\epsilon_{\sigma}(\bar{\lambda})$, $\epsilon_{\omega}(\bar{\mu})$, and $\epsilon_{\tau}(\bar{\nu})$ are given by Eq. (15), and $p_{\sigma}(\bar{\lambda})$, $p_{\omega}(\bar{\mu})$, and $p_{\tau}(\bar{\nu})$ are given by Eq. (16). The energy-momentum dispersion of various magnon types of excitations are plotted in Fig. 2. In the spectrum calculations, we have used the periodicity in momentum P, so that $\Delta E(P+2\pi) = \Delta E(P)$. For instance, for the 45-fold degenerate states, $\Delta E_{(45)}(P) = \epsilon_{\sigma}(q_1) + \epsilon_{\sigma}(q_2) + \epsilon_{\omega}(q_3)$, where $P = q_1 + q_2 + q_3$, with modula 2π . In a recent paper in Ref. 15, the lower-lying excitations of model (1) were calculated numerically for finite systems. Their results are consistent with ours in Fig. 2. In particular, both the numerical calculations and the present Bethe ansatz solutions show the following feature: as the momentum |p| increases from 0 to π , the lowest excitations are changed from the 15-fold degenerate states to the 45-fold degenerate states at $|P| = \pi/2$.



FIG. 3. (a) A $\langle S_j T_j \rangle$ staggeringly ordered state to demonstrate the ground state, the SU(4) singlet, (b) flavorons of one σ type and one τ type compounded symmetrically to form a 15-fold multiplet, and (c) compounded antisymmetrically to form a singlet. (d) The 20-fold multiplet being compounded of two flavorons of ω type. (e) The 45-fold multiplet being compounded of two flavorons of σ type and one flavorons of ω type. (f) The 35-fold multiplet being compounded of four flavorons of σ type.

In Fig. 3, we illustrate these generalized magnon types of composite low-lying excited states. We start with a typical configuration of the ground state in Fig. 3(a), and the various generalized magnon excitations are created from the ground state by introducing two or more flavorons as shown in Figs 3(b)–(f), which arise from various possible flips of spin or orbital or both. The flavoron indicated by the dashed box in Fig. 3 moves in the background of the SU(4) singlet carrying both energy and the quantum numbers. The σ -type (flavoron) excitation mode is a moving quaduplet with $|\uparrow_{-}\rangle$ being the local highest weight state. The ω -type excitation mode is a moving dust here is a moving quaduplet with $|\uparrow_{-}\rangle - |\downarrow_{-}\uparrow\rangle - |\downarrow_{-}\uparrow\rangle + |\uparrow_{-}\uparrow\rangle - |\uparrow_{-}\uparrow\rangle$ being the local highest weight state.

VI. SUMMARY

In this paper we have used the Bethe ansatz method to discuss extensively the ground state and various types of the low-lying excited states of a Heisenberg spin chain with two-fold orbital degeneracy in the limit of SU(4) symmetry. There are three types of elementary excitations in the present model. Two of them carry spin 1/2 and orbital 1/2, and both are fourfold degenerate. The third one carries either spin 1 or orbital 1, and is sixfold degenerate. We have constructed magnon types of composite excitations and calculated their spectra.

ACKNOWLEDGMENTS

Y.Q.L. acknowledges Grant Nos. NSFC-19675030 and NSFZ-198024 and support from the Y. Pao & Z. Pao Foundation. The work is supported in part by DOE Grant No. DE/FG03-98ER45687. We thank G. S. Tian for a reference.

- ¹D. B. McWhan, T. M. Rice, and J. P. Remeika, Phys. Rev. Lett.
 23, 1384 (1969); D. B. McWhan, A. Menth, J. P. Remeika, W. F. Brinkman, and T. M. Rice, Phys. Rev. B 7, 1920 (1973).
- ²C. Castellani, C. R. Natoli, and J. Ranninger, Phys. Rev. B 18, 4945 (1978); 18, 4967 (1978); 18, 5001 (1978).
- ³R. E. Word, S. A. Werner, W. B. Yelon, J. M. Honig, and S. Shivashankar, Phys. Rev. B 23, 3533 (1981).
- ⁴K. I. Kugel and D. I. Khomskii, Usp. Fiz. Nauk 136, 621 (1982),
 [Sov. Phys. Usp. 25, 231 (1982)].
- ⁵W. Bao, C. Broholm, S. A. Carter, T. F. Rosenbaum, G. Aeppli, S. F. Trevino, P. Metcalf, J. M. Honig, and J. Spalek, Phys. Rev. Lett. **71**, 766 (1993).
- ⁶ T. M. Rice, in *Spectroscopy of Mott Insulators and Correlated Metals*, edited by A. Fujimori and Y. Tokura (Springer, Berlin, 1995).
- ⁷H. F. Pen, J. van den Brink, D. I. Komomskii, and G. A. Sawatzky, Phys. Rev. Lett. **78**, 1323 (1997).
- ⁸K. Yamaura, M. Takano, A. Hirano, and R. Kanno, J. Solid State Chem. **127**, 109 (1997), and references therein.
- ⁹S. Ishihara, J. Inoue, and S. Maekawa, Phys. Rev. B **55**, 8280 (1997); S. Ishihara, M. Yamanaka, and N. Nagaosa, *ibid.* **56**, 686 (1997).
- ¹⁰R. Shiina, T. Nishitani, and H. Shiba, J. Phys. Soc. Jpn. **66**, 3159 (1997).
- ¹¹L. F. Feiner, A. M. Oles, and J. Zaanan, Phys. Rev. Lett. **78**, 2799 (1997).

- ¹²D. P. Arovas and A. Auerbach, Phys. Rev. B **52**, 10 114 (1995).
- ¹³A. Onufriev and J. B. Marston, Phys. Rev. B **59**, 12 573 (1999).
- ¹⁴Y. Q. Li, M. Ma, D. N. Shi, and F. C. Zhang, Phys. Rev. Lett. 81, 3527 (1998).
- ¹⁵Y. Yamashita, N. Shibata, and K. Ueda, Phys. Rev. B 58, 9114 (1998).
- ¹⁶B. Frischmuth, F. Mila, and T. M. Rice (private communication).
- ¹⁷V. L. Pokrovskii and G. V. Uimin, Zh. Éksp. Teor. Fiz. **61**, 859 (1971) [Sov. Phys. JETP **34**, 457 (1972)].
- ¹⁸B. Sutherland, Phys. Rev. B **12**, 3795 (1975); Phys. Rev. Lett. **20**, 98 (1968).
- ¹⁹E. Wigner, Phys. Rev. **51**, 1069 (1937).
- ²⁰L. Faddeev and L. Takhtajan, Phys. Lett. 80A, 375 (1981).
- ²¹E.g., R. Gilmore, *Lie Groups, Lie Algebras and Some of their Applications* (John Wiley & Sons, New York, 1974).
- ²²I. Affleck and E. Lieb, Lett. Math. Phys. **12**, 57 (1986); I. Affleck, Phys. Rev. B **37**, 5186 (1988), and private communications.
- ²³E. Lieb, T. Schulz, and D. Mattis, Ann. Phys. (N.Y.) 16, 407 (1961).
- ²⁴H. Bethe, Z. Phys. **75**, 205 (1931); J. H. Lowenstein, in *Recent Advances in Field Theory and Statistical Mechanics*, edited by J. Zuber and R. Stora (Elsevier, Amsterdam, 1884), p. 612.
- ²⁵F. Woynarovich, J. Phys. C **15**, 85 (1982); **15**, 97 (1982).
- ²⁶D. C. Mattis, *The Theory of Magnetism I* (Springer-Verlag, Berlin, 1981).