Effective chiral-spin Hamiltonian for odd-numbered coupled Heisenberg chains

V. Subrahmanyam

International Center for Theoretical Physics, P.O. Box 586, 34100 Trieste, Italy

(Received 7 September 1994)

An $L \times \infty$ system of an odd number of coupled Heisenberg spin chains is studied using a degenerate perturbation theory, where L is the number of coupled chains. An effective chain Hamiltonian is derived explicitly in terms of two spin-$\frac{1}{2}$ degrees of freedom of a closed chain of L sites, valid in the regime where the interchain coupling is stronger than the intrachain coupling. The spin gap has been calculated numerically using the effective Hamiltonian for $L = 3$, 5, 7, and 9 for a finite chain up to ten sites. It is suggested that the ground state of the effective Hamiltonian is correlated, by examining various variational trial states for the effective-spin chain Hamiltonian.

There is a growing interest in coupled chains of Hubbard-Heisenberg spin systems, following the experimental realization of coupled arrays of metal-oxide-metal ladder systems.[1,2] A number of investigations[3–7] of weakly coupled Heisenberg spin chains have been carried out, in which the coupling between the chains is weaker than the intrachain coupling, and have provided a strong indication that a system with an even number of chains can be understood in terms of a short-range resonating-valence-bond (RVB) picture, with spin gap and a finite spin-spin correlation length. Conversely, a system with an odd number of chains is gapless with power-law spin correlations, indicating that it is in the same universality class as a single spin chain. The framework for understanding the difference between even- and odd-numbered chains is the RVB picture,[6,8] which suggests that an even-numbered coupled-chain system can be thought of as an integer spin chain exhibiting a Haldane spin gap, and an odd-numbered coupled system maps onto a half-odd-integer spin chain. Below we will construct an effective-spin Hamiltonian for an odd-numbered coupled system, which is cast explicitly in terms of spin-$\frac{1}{2}$ degrees of freedom. This can be done straightforwardly in the regime where the coupling along the chain is weaker than the coupling between the chains, complementary to the earlier studies.

We consider the Heisenberg Hamiltonian given as

$$H = J \sum_{l,n} \vec{s}_{l,n} \cdot \vec{s}_{l+1,n} + J' \sum_{l,n} \vec{s}_{l,n} \cdot \vec{s}_{l,n+1} - h \sum_{l,n} s_{l,n}^z \quad (1)$$

defined on an $L \times N$ lattice where $l = 1, 2, \ldots, L$ and $n = 1, 2, \ldots, N$, and $\vec{s}_{l,n}$ is a spin-1/2 operator at site (l,n). The intrachain exchange coupling constant is J' and the interchain coupling constant is J, and h is a magnetic field. We use periodic boundary conditions in both directions, and as we see below it makes a big difference. We are interested in the regime where $J' < J$, and the case of odd-numbered coupled chains, $L = 3, 5, \ldots$. We can think of the system as consisting of N sites with 2^L degrees of freedom at each site, and a complicated bond interaction between the sites mediated by the J' bonds in the Hamiltonian given above. Starting with an unperturbed system with $J' = 0$, we proceed to include the effect of a nonzero J' within perturbation theory. This is achieved by identifying the most relevant degrees of freedom for a given site, and projecting out the not so important degrees of freedom. Below we explicitly show an analytical construction of the effective-spin chain Hamiltonian for the case of $L = 3$ and 5, and for a larger L one can perform a similar procedure numerically.

Let us consider the case of $J' = 0$, and $h = 0$. The ground state of the system is the direct product of N copies of the ground state of a closed chain with L sites. The ground state of the Heisenberg Hamiltonian of a closed chain with an odd number of sites is in the sector with total spin $S = \frac{1}{2}$ and $S^z = \pm \frac{1}{2}$, implying at least a twofold Kramers degeneracy. As a matter of fact, the ground state is fourfold degenerate. This extra degeneracy arises from chirality. This can be viewed as an unpaired spin in an otherwise singlet ground state, i.e., a spinon which is forced to be there in the ground state.[9] In addition to the spin, the spinon carries a finite ground-state momentum $\pm 4\pi/L$ (orbital angular momentum about the center of the closed chain). In the case of an open chain the chiral degeneracy disappears, and we will be left with a twofold Kramers-degenerate ground state with $S^z = \pm 1/2$. The two ground states in the $S^z = \frac{1}{2}$ sector can be written as $\phi_{1/2,\pm}^L = \Sigma a_\pm^L(\{n_i\}) | \{n_i\} \rangle$, where n_i refer to locations of down spins $(n_1 < n_2 \ldots)$. Similarly the ground states in the $S^z = -\frac{1}{2}$ sector can be written (here n_i refer to the up spins). The amplitudes $a_\pm^L$ are found using a Bethe ansatz;[10] for $L = 3$ the amplitudes are given by (there is only one down spin in this case) $a_\pm^3(n_1) = \exp(\pm i2\pi n_1/3)$, and for $L = 5$ the amplitudes are given by (there are two down spins in this case)

$$a_\pm^5(n_1, n_2) = \exp[\pm 2ik(n_1 + n_2)] \cos[(k - \eta/5)(n_2 - n_1) + \eta/2], \quad (2)$$

where $k = 2\pi/5$ and the phase shift $\eta = 2.243 \ldots$. These two different states have spin currents going in two different directions. We refer to these two states as having chirality by defining $\chi^z | \phi_\pm^L \rangle = \pm \frac{1}{2} | \phi_\pm^L \rangle$, and the associated raising and lowering operators through $\chi^\pm | \pm \rangle = 0$, $\chi^\pm | \mp \rangle = | \pm \rangle$. The

chirality operator $\vec{\chi}$ can be written in terms of the original spin operators. Following Ref. 11, we define a permutation operator P_l at a site l which permutes the spin labels such that $l+m \rightarrow N+l-m$. This is equivalent to doing a reflection on a regular polygon with L sites, around a straight line bisecting the angle at site l. The P operators can be readily constructed from the spin operators, as each of them involve $(L-1)/2$ pairwise permutations, as $P_l=2^{(N-1)/2}\Pi_{m=1}^{(N-1)/2}(\vec{s}_{l+m}\cdot\vec{s}_{N+l-m}+\frac{1}{4})$. Also, P_l can be expressed in terms of chiral lowering and raising operators as $P_l=A_l^*\chi^+ + A_l\chi^-$, where $A_l=\exp(i2\pi l/L)$. The chirality operator is now related to the original spin operators through $[P_l,P_{l+m}]=4i\chi^z\sin2\pi m/L$, and $\chi^x=P_1/2$.

If we denote the gap in the spectrum for this L-site closed chain by δ_L (see Table I for the actual values of the gap for $L=3$, 5, 7, and 9), for $J'<\delta_L$ it is a good approximation to just keep the ground-state manifold, 4^N-fold degenerate for $J'=0$, and drop the excited states. This is expected to suffice for understanding the low-energy behavior of the system described by the Hamiltonian given in Eq. (1), as the excitation processes that include the states dropped have high energy. The ground-state subspace we keep, belonging to the spin-1/2 sector of each site (of 2^L states), is identified as the most relevant degrees of freedom. For $L=3$, this procedure keeps all the spin-1/2 states at each site. However, for larger $L>3$, there are also spin-1/2 excited states with large energy which are eliminated in our procedure. This approximation is not so good for $L=9$ or more, as the range of J' for validity of our procedure becomes very restricted, viz. $J'<0.8612$ for $L=9$. The ground-state subspace for $J'=0$ is only 2^N-dimensional if we use open boundary conditions for the L-site chain; in contrast for periodic boundary conditions we get a much larger Hilbert space, rendering the perturbation theory to be valid in a smaller regime of J' as the gap for the L-site open chain is smaller than that of a closed chain. Each of the basis states ψ_i for the full system is a direct product of N ground-state eigenfunctions of a close chain of L sites. $\psi_i=\phi_{l_1}^1\times\phi_{l_2}^2\cdots\times\phi_{l_N}^N$, where $l_i=1,4$. To find the effective Hamiltonian within this subspace, we compute the matrix elements $\langle\psi_i|H'|\psi_j\rangle$, and use them to construct an effective Hamiltonian. The prime denotes that only J' bonds are included. The evaluation of the matrix elements reduces to a two-site problem (actually two closed chains of length L connected by L bonds of strength J') as we have pairwise interactions only.

Let us use two spin-$\frac{1}{2}$ effective degrees of freedom for constructing an effective Hamiltonian, the spin and the chiral quantum numbers $\vec{S}_i$ and the chirality $\vec{\chi}_i$ of the L-site closed chains. An explicit calculation shows that the effective interaction strength $\vec{A}_{i,j}$ between two closed chains connected by a J' bond (the corresponding operator is $\vec{s}_{i,1}\cdot\vec{s}_{j,2}$) at sites i and j is given in terms of the total spins of the two closed chains and the permutation operators, which we discussed above, at sites i and j, respectively, of two chains as

$$\vec{A}_{i,j}=J'\alpha_L\vec{S}_1\cdot\vec{S}_2\left(\gamma_L+\frac{P_i(1)}{2}\right)\left(\gamma_L+\frac{P_j(2)}{2}\right). \quad (3)$$

Here for $L=3$, $\alpha_3=16/9$, $\gamma_3=1/4$, and for $L=5$ $\alpha_5=16\beta$, $\gamma_5=1/20\sqrt{\beta}$. The parameter β is given in terms of $x_1=\cos k-\eta/5+\eta/2$, and $x_2=\cos2(k-\eta/5)+\eta/2$ as

TABLE I. The energy gap of an L-site ring, and the wave-function renormalization constants that appear in the effective Hamiltonian given in Eq. (5) for various values of L.

L	δ_L/J	b_L	K_L/J'
3	3/2	1/8	8/3
5	1.1180	0.0697	2.8685
7	1.0489	0.0436	3.2765
9	0.8612	0.0230	4.8275

$$\beta=\frac{2}{5}\frac{(1+\cos2k)x_1^4+(1+\cos k)x_2^4-x_1^2x_2^2}{x_1^2+x_2^2}. \quad (4)$$

For $L>5$, the wave-function renormalization constants α_L and γ_L are difficult to calculate analytically, as the number of s^z-basis states in $S^z=1/2$ becomes very large. However, the constants can be calculated numerically, and the form of the interaction remains valid. Numerically computed values of the constants are given in Table I for up to $L=9$.

The interaction H'_{12} between two closed chains is mediated by L bonds of strength J', $H'_{12}=J'\Sigma_i\vec{s}_{i,1}\cdot\vec{s}_{i,2}$, which in terms of the effective degrees of freedom is obtained by $\Sigma_i\vec{A}_{i,i}$. Now it is straightforward to write the effective Hamiltonian for the full system within the closed-chain ground-state subspace as

$$H_{\text{eff}}=K_L\sum_{i=1}^{N}\vec{S}_i\cdot\vec{S}_{i+1}(b_L+\chi_i^x\chi_{i+1}^x+\chi_i^y\chi_{i+1}^y), \quad (5)$$

where $K_L=J'\alpha_L L/2$, and $b_L=2\gamma_L^2$ ($K_3=8J'/3$, $b_3=1/8$, and $K_5\approx2.845J'$, $b_5\approx0.06528$, see Table I). It is interesting to note that only the xy component of the chiral interaction enters the effective Hamiltonian leaving only a twofold up-down symmetry for the chiral variables. The rotational invariance for the total spin is expected as we started with a fully rotational invariant interaction and we did not break the symmetry by restricting the Hilbert space to the spin-1/2 sector of every closed chain. Just by looking at the form of the effective interaction we learn that on a pair of neighboring sites the spins and chiral variables are strongly correlated. If we try to lower the spin energy by forcing a singlet state between a pair of neighboring sites, the chiral variables go into a triplet state (with $\chi^z=0$). However, because of the additive constant b_L in front of the chirality interaction, a spin triplet and a chiral singlet are not favored.

Let us try some variational ansatz. A simple variational state of spin singlets and chiral triplets on nearest neighbors, $\psi_{ST}=\Pi_{i\,\text{odd}}\psi_i^S\psi_i^T$, where ψ_i^S is a spin singlet between sites i and $i+1$ and ψ_i^T is a chiral triplet state with $\chi^z=0$, gives an upper bound on the ground-state energy of the effective Hamiltonian given above $E_{\text{eff}}^G/K_L\leq E_{ST}(2)/K_L=-\frac{3}{4}(b_L+\frac{1}{2})N/2$ ($=-0.9375N/4$, for $L=3$). The factor $-\frac{3}{4}$ is the spin singlet energy, 1/2 is the chiral triplet energy, and $N/2$ is due to the fact that only half the bonds have spin singlets and chiral triplets. This state is of course too simple to give us any insight about the structure of the actual ground state. However, as we will see below, it is doing better than

expected. Let us use Jordan-Wigner fermion language for the chirality terms. The xy term translates into a simple spinless fermion hopping. Now it is tempting to try a free fermion ground state for chirality variables, with an average value of $1/\pi$ for the xy chiral interaction. In this case, we would be left with a Bethe ansatz ground state for the spins, giving an energy estimate $E_{BF}/K_L=-(\ln 2-\frac{1}{4})(b_L+1/\pi)$ $\times N(\approx -0.786N/4$ for $L=3)$. Compared to the singlet-triplet valence bond variational state the Bethe free-fermion variational state has 20% larger energy, indicating that a correlated state with spin singlets and chiral triplets with longer-ranged valence bonds would do much better. Let us consider a four-site system and construct valence-bond state space. We form two orthogonal states for a four-site system (the sector with $S=0$ has only two states in this case) from the valence bond states, viz., $A=(12)(34)$, $B=\{(23)(41)$ $-\frac{1}{2}(12)(34)\}2/\sqrt{3}$, where (12) stands for a spin singlet between the two sites. Similarly we construct the chiral states A' and B' where (12) denotes a chiral triplet with $\chi^z=0$. Diagonalizing the effective Hamiltonian given in Eq. (5), with this fourfold spin-chiral valence bond subspace, yields a variational energy of $E_{ST}(4)/K_L\approx -0.9695N/4$ for $L=3$. This is a 3% lowering of energy compared to the nearest-neighbor valence bond state we considered above. The probability amplitude for a valence bond configuration with a bond occupied by a spin singlet and chiral triplet is more than the other configurations, implying strong correlations between the spin and chiral degrees of freedom. It is interesting to note that this further-neighbor valence bond variational state has an energy very close to the exact ground-state energy by less than 3% (the indication from numerical diagonalization of the effective Hamiltonian on a finite site system up to $N=10$ is that the ground-state energy tends to $-NK_L/4$ for $L=3$, as we discuss below).

An effective way of constructing a convergent series of upper bounds on the exact ground-state energy is by calculating the ground-state energy $E(n)$ of a finite open chain of n-$even$ sites, giving rise to a variational inequality $E_G/N\leq E(n)/n$. The best bound is obtained from the largest open chain that can be numerically diagonalized. Since the number of states per site is 4, we are able diagonalize only up to ten sites. This gives us a bound for $L=3$

$$E_{GS}/NK_3 \leq E(10)/10 \approx -0.9932/4. \tag{6}$$

From this calculation it seems that the ground-state energy is tending towards $-NK_L/4$ from above. Similarly one can construct a sequence of lower bounds variationally from the l-site chain energy through $E_G/N\geq E(n)/(n-1)$. However, this sequence is seen to be not as convergent as the sequence of upper bounds. A better convergent sequence of lower bounds can be constructed by varying the bond strengths for a given n-site chain, which becomes very complicated for even $n=6$, and we will not present the details here. The ground state is seen to be in a sector with $S=0$ and $\chi^z=0$, in all the finite chain diagonalizations we have done up to $N=10$. The spin gap, defined as the difference between the energies of the lowest-energy states of the sector $S=1,\chi^z=0$ and $S=0,\chi^z=0$, is seen to fall off as the number of sites is increased, as shown in Fig. 1, for different values of L. However, the data at hand are insufficient to fit the
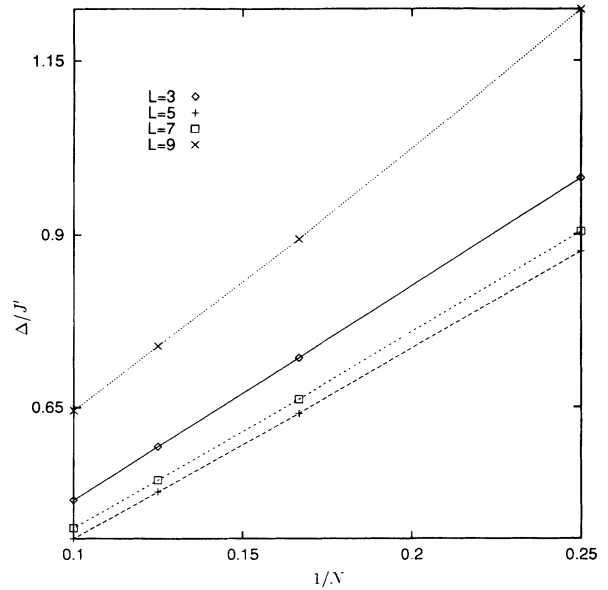

FIG. 1. The spin gap of an $L\times N$ system as a function of $1/N$ for various numbers of coupled chains, $L=3$, 5, 7, and 9. The gap is calculated numerically from the effective Hamiltonian given in Eq. (5).

finite-N scaling of the gap. The gap seems to be nonmonotonic as a function of L for a given value of N; as can be seen from the figure for $L=9$ the gap is larger than for $L=3$. This could be an artifact of our approximation, implying the perturbation theory in conjunction with the truncation we have implemented may not be valid for larger L. We have studied the spin-spin correlation function also for the ten-site chain and is seen to be slowly decaying as in the case of $L=1$. We may conjecture that the decay is likely to be slower for a larger L than that for the case of $L=1$, though we are not able to substantiate it just now. This is based on the fact that we have a long-ranged valence bond ground state, and the probability amplitude for a configuration with a valence bond between two sites far apart would be much smaller for a larger L than for the case of $L=1$. But the characterization of the long-distance behavior needs an investigation of larger chains. The density matrix renormalization approach[8] can be used for this; currently an investigation is in progress incorporating this scheme for the finite-size spectrum and thermodynamics of larger chains ($N>10$) for the effective Hamiltonian.

Now we consider the case of a nonzero magnetic field in the Hamiltonian given in Eq. (1). It is easy to see that the effective Hamiltonian given in Eq. (5) will have an additional piece, viz., $-h\Sigma S_i^z$. Let us focus on the case of $L=3$. The effective Hamiltonian is valid in the regime $h<3J/4$, for $L=3$, to ensure that the ground-state subspace is composed of $S^z=\pm 1/2$ states of the L-site chains. Now, if the magnetic field is strong enough to polarize the spins in the effective Hamiltonian, the ground state would be just a polarized spin and a free fermion state for the chiral degrees of freedom. The range of h for which this state has lower energy than the $S=0$ state works out to be for $0.75J>h>(7\pi-8)J'/6\pi\approx 0.74225J'$. The free fermion chiral state has low-lying excited states with a gap of

$\Delta = (7\pi - 8)K_3/4N$. This should be contrasted with the case of $L = 1$, where there are no low-lying states if the magnetic field is of the order of the exchange coupling constants.

In conclusion, we have established an effective spin-chiral chain Hamiltonian for a system of odd-numbered coupled Heisenberg spin chains. The effective interaction has a product form, viz., an isotropic Heisenberg for spins and only xy interaction for chiral spins. The spin gap studied numerically using the effective Hamiltonian for $L = 3, 5, 7$, and 9 falls off as the number of sites i increases. Indications from a finite-size study are that long-ranged resonating-valence-bond variational states (with spin singlets and chiral triplets) are suited for studying the behavior of the effective Hamiltonian.

[1] D. C. Johnston et al., Phys. Rev. B **35**, 219 (1987).

[2] M. Takano, Z. Hirori, M. Azuma, and Y. Takeda, Jpn. J. Appl. Phys. **7**, 3 (1992).

[3] E. Dagotto, J. Riera, and D. J. Scalapino, Phys. Rev. B **45**, 5744 (1992).

[4] S. P. Strong and A. J. Millis, Phys. Rev. Lett. **69**, 2419 (1992).

[5] T. Barnes et al., Phys. Rev. B **47**, 3196 (1993); Phys. Ser. **7**, 3 (1992).

[6] T. M. Rice, S. Gopalan, and M. Sigrist, Europhys. Lett. **23**, 445 (1993).

[7] A. Parola, S. Sorella, and Q. F. Zhong, Phys. Rev. Lett. **71**, 4393 (1993).

[8] S. R. White, R. M. Noack, and D. J. Scalapino, Phys. Rev. Lett. **73**, 886 (1994).

[9] L. A. Takhatajan and L. D. Faddeev, Phys. Lett. **85A**, 375 (1981).

[10] R. B. Griffiths, Phys. Rev. **133**, A768 (1964).

[11] V. Subrahmanyam, Phys. Rev. B **50**, 6468 (1994).