

## Strong-Coupling Expansions for Multiparticle Excitations: Continuum and Bound States

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We present a new linked cluster expansion for calculating properties of multiparticle excitation spectra to high orders. We use it to obtain the two-particle spectra for systems of coupled spin-half dimers. We find that even for weakly coupled dimers the spectrum is very rich, consisting of many bound states. The number of bound states depends on both geometry of coupling and frustration. Many of the bound states can only be seen by going to sufficiently high orders in the perturbation theory, showing the extended character of the pair attraction.

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The study of bound states, lifetimes, and spectral weights for multiparticle excitations remains a challenging problem in many-body physics. From an experimental point of view, a variety of probes on several low-dimensional magnetic and strongly correlated electronic systems shows spectral features associated with multiparticle continuum and bound states. These features in two-magnon Raman spectra, optical absorption spectra, photoemission, and even in neutron scattering spectra remain poorly understood. From a theoretical point of view, one of the most intriguing issues is the role the growing number of bound states play in the confinement-deconfinement transition in spin-Peierls systems as the spectrum completely changes from soliton-antisoliton continuum to triplets, their bound states, and continuum [1]. Existing computational approaches to these problems are not adequate.

In this Letter, we present significant advances in calculating multiparticle spectral properties from high-order strong-coupling expansions. At the heart of our method is a generalization of Gelfand's linked cluster expansion for single-particle excited states [2] to multiparticle states. From a technical point of view, our most notable achievement is the development of an orthogonality transformation which leads to a linked cluster theorem for multiparticle states even with quantum numbers identical to the ground state. Our method is quite distinct from the flow equation method of Wegner [3], which has been used recently by Knetter *et al.* [4] for also studying multiparticle spectral properties, but for a more restricted class of models with equispaced unperturbed eigenvalues.

We apply our method to systems of coupled spin-half dimers in various one- and two-dimensional geometries. The calculations greatly simplify when we deal with models where the ground state is known exactly to be a product of dimers, such as the Shastry-Sutherland models in one and two dimensions [5]. Here, we focus attention on the one-dimensional systems. Results are presented for a spin-ladder system, the alternating spin-chain model, and the Shastry-Sutherland model.

Except for the spin-ladder model, the high-order calculations produce qualitatively unexpected results. There are multiple bound states with  $S = 0, 1,$  and  $2$  even in the weakly coupled dimer limit. The number of bound states varies with frustration and many of them show up only when the expansions are done to sufficiently high order. This presumably is due to the extended range of the attractive interaction needed to see the multiple bound states. The interval of  $k$  values where the bound states exist also changes with the coupling of the dimers.

We begin describing our method with a Hamiltonian

$$H = H_0 + \lambda H_1, \quad (1)$$

where the unperturbed part  $H_0$  is exactly solvable, and  $\lambda$  is the perturbation parameter. The aim is to calculate perturbation series in  $\lambda$  for the eigenvalues of  $H$  and other quantities of interest. As is well known [6,7], the ground-state energy and correlation functions have a "cluster addition property" and hence can be calculated by linked cluster expansion.

We wish to consider the excited-state many-particle sectors of the Hilbert space, where a "particle" may refer to a lattice fermion, a spin flip, or other excitation, depending on the model at hand. The key step is to "block diagonalize" the Hamiltonian on any finite cluster to form an effective Hamiltonian, via an orthogonal transformation (here we will consider only real Hamiltonians):

$$H^{\text{eff}} = O^T H O, \quad (2)$$

where  $O = e^S$  and  $S$  is real, antisymmetric. This transformation is constructed order by order in perturbation theory, so that the ground state sits in a block by itself, the one-particle states (which form a degenerate manifold under  $H_0$ , in general) form another block, the two-particle states another block, and so on. The off-diagonal blocks of  $S$  are determined by the requirement that the off-diagonal blocks of  $H^{\text{eff}}$  vanish, and we choose the diagonal blocks of  $S$  to be zero.

Let the matrix element of  $H^{\text{eff}}$  between initial one-particle state  $|\mathbf{i}\rangle$  and final one-particle state  $|\mathbf{j}\rangle$ , labeled according to their positions on the lattice, be

$$E_1(\mathbf{i}, \mathbf{j}) = \langle \mathbf{j} | H^{\text{eff}} | \mathbf{i} \rangle. \quad (3)$$

This excited-state energy is not extensive, and does not obey the cluster addition property. However, as shown by Gelfand [2], the “irreducible” one-particle matrix element

$$\Delta_1(\mathbf{i}, \mathbf{j}) = E_1(\mathbf{i}, \mathbf{j}) - E_0 \delta_{\mathbf{i}, \mathbf{j}} \quad (4)$$

does have the cluster addition property. Furthermore, for a translationally invariant system, the one-particle states are eigenstates of momentum:

$$|\mathbf{K}\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{j}} \exp(i\mathbf{K} \cdot \mathbf{j}) |\mathbf{j}\rangle \quad (5)$$

(where  $N$  is the number of sites in the lattice), with energy above the ground state of

$$\omega_1(\mathbf{K}) = \sum_{\delta} \Delta_1(\delta) \cos(\mathbf{K} \cdot \delta). \quad (6)$$

To generalize to two-particle states, let

$$E_2(\mathbf{i}, \mathbf{j}; \mathbf{k}, \mathbf{l}) = \langle \mathbf{k}, \mathbf{l} | H^{\text{eff}} | \mathbf{i}, \mathbf{j} \rangle \quad (7)$$

be the matrix element between initial two-particle state  $|\mathbf{i}, \mathbf{j}\rangle$  and final state  $|\mathbf{k}, \mathbf{l}\rangle$ . To obtain a quantity obeying

$$(E - E_0)f_{ij} - \sum_{\mathbf{k}} [\Delta_1(\mathbf{k}, \mathbf{i})f_{kj} + \Delta_1(\mathbf{k}, \mathbf{j})f_{ik}] = \frac{1}{2} \sum_{\mathbf{k}, \mathbf{l}} \Delta_2(\mathbf{k}, \mathbf{l}; \mathbf{i}, \mathbf{j})f_{kl} - \Delta_1(\mathbf{j}, \mathbf{i})f_{jj} - \Delta_1(\mathbf{i}, \mathbf{j})f_{ii}, \quad \text{all } \mathbf{i}, \mathbf{j}. \quad (10)$$

The fictitious amplitudes  $f_{ii}$  are *defined* by these equations [8], and are introduced to simplify the Fourier transform. Defining the center-of-mass momentum  $\mathbf{K}$  and the relative momentum  $\mathbf{q}$ , this can be turned into an integral equation:

$$\begin{aligned} & \left[ E - E_0 - 2 \sum_{\delta} \Delta_1(\delta) \cos(\mathbf{K} \cdot \delta/2) \cos(\mathbf{q} \cdot \delta) \right] f(\mathbf{K}, \mathbf{q}) \\ &= \frac{1}{N} \sum_{\mathbf{q}'} f(\mathbf{K}, \mathbf{q}') \left[ \frac{1}{2} \sum_{\mathbf{r}, \delta_1, \delta_2} \Delta_2(\mathbf{r}, \delta_1, \delta_2) \cos(\mathbf{K} \cdot \mathbf{r}) \cos(\mathbf{q} \cdot \delta_1) \times \cos(\mathbf{q}' \cdot \delta_2) - 2 \sum_{\delta} \Delta_1(\delta) \cos(\mathbf{K} \cdot \delta/2) \cos(\mathbf{q} \cdot \delta) \right], \end{aligned} \quad (11)$$

which can be solved by standard numerical techniques like discretization. The spectrum of the discretized Hamiltonian can be obtained by diagonalization. In this way the spectrum and even the two-particle density of states can be obtained. The continuum is limited by the the maximum (minimum) of the energy of two single-particle excitations whose combined momentum is the center-of-mass momentum, which serves as an independent check.

We have used this method to investigate the low-energy excitation spectrum of the two-leg spin- $\frac{1}{2}$  Heisenberg ladder

$$H = \sum_i [J\mathbf{S}_i \cdot \mathbf{S}_{i+1} + J\mathbf{S}'_i \cdot \mathbf{S}'_{i+1} + J_{\perp}\mathbf{S}_i \cdot \mathbf{S}'_i], \quad (12)$$

where the interactions along the ladder ( $J$ ) and along the rungs ( $J_{\perp}$ ) are assumed to be antiferromagnetic.

For  $J/J_{\perp} < \infty$ , the ground state of this model evolves smoothly from a product of singlet states along the rungs of the ladder and has a gapped excitation spectrum [9–11].

the cluster addition property, we must subtract the ground-state energy and one-particle contributions to form the irreducible two-particle matrix element:

$$\begin{aligned} \Delta_2(\mathbf{i}, \mathbf{j}; \mathbf{k}, \mathbf{l}) &= E_2(\mathbf{i}, \mathbf{j}; \mathbf{k}, \mathbf{l}) - E_0(\delta_{\mathbf{i}, \mathbf{k}}\delta_{\mathbf{j}, \mathbf{l}} + \delta_{\mathbf{i}, \mathbf{l}}\delta_{\mathbf{j}, \mathbf{k}}) \\ &\quad - \Delta_1(\mathbf{i}, \mathbf{k})\delta_{\mathbf{j}, \mathbf{l}} - \Delta_1(\mathbf{i}, \mathbf{l})\delta_{\mathbf{j}, \mathbf{k}} \\ &\quad - \Delta_1(\mathbf{j}, \mathbf{k})\delta_{\mathbf{i}, \mathbf{l}} - \Delta_1(\mathbf{j}, \mathbf{l})\delta_{\mathbf{i}, \mathbf{k}}. \end{aligned} \quad (8)$$

This quantity is easily found to be *zero* for any cluster unless  $\mathbf{i}$ ,  $\mathbf{j}$ ,  $\mathbf{k}$ , and  $\mathbf{l}$  are all included in that cluster, and it obeys the cluster addition property. The block diagonalization ensures that two particles cannot “annihilate” from one cluster and “reappear” on another disconnected one. Thus the matrix elements of  $\Delta_2$  can be expanded in terms of connected clusters alone, which are rooted or connected to all four positions  $\mathbf{i}$ ,  $\mathbf{j}$ ,  $\mathbf{k}$ , and  $\mathbf{l}$ .

Once the effective two-particle Hamiltonian is known, we still have to solve the Schrödinger equation. Consider for simplicity a two-particle state of identical particles, or one symmetric under particle exchange. Then expand the two-particle eigenstate

$$|\psi\rangle = \sum_{\mathbf{i} > \mathbf{j}} f_{ij} |\mathbf{i}, \mathbf{j}\rangle, \quad f_{ij} = f_{ji}, \quad (9)$$

and the Schrödinger equation takes the form

The occurrence of two-particle bound states in this model has been shown by first-order strong-coupling expansions [12,13] as well as a leading order calculation using the analytic Brueckner approach [14,15].

Starting from the dimerized ground state we have calculated series in  $J/J_{\perp}$  for  $\Delta_2$  up to order 7 for singlet states, and to order 12 for triplet and quintet states [16]. Figure 1 shows the generic shape of the two-particle continuum as well as the low-lying massive excitations. Beside the elementary triplet excitation the spectrum shows additional singlet ( $S = 0$ ) and triplet ( $S = 1$ ) excitations which are bound states of two elementary triplets. In the vicinity of  $K \approx \pi$  there is also an  $S = 2$  antibound state above the continuum. At  $J/J_{\perp} = 1/2$ , we find the binding energy for the singlet bound state at  $K = \pi$  is  $E_b/J_{\perp} = 0.51$ , substantially larger than the value 0.35 obtained in [15].

Further, we have studied the occurrence of bound states in the alternating Heisenberg chain,

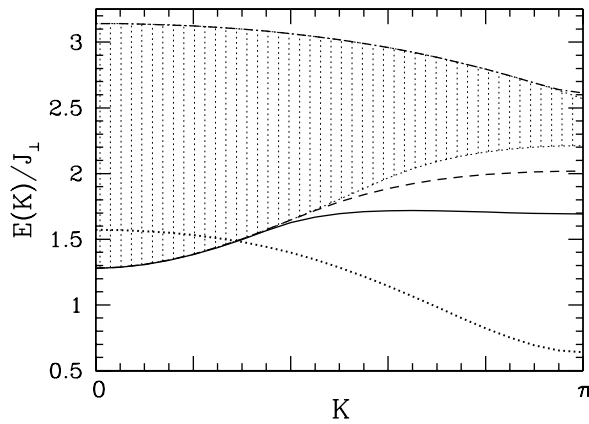


FIG. 1. Low-energy excitation spectrum of the Heisenberg spin ladder for  $J/J_{\perp} = 1/2$ . Beside the two-particle continuum (gray shaded) and the elementary triplet excitation (dotted line) there are three massive quasiparticles: a singlet bound state (solid line), a triplet bound state (dashed line), and a quintet antibound state (dash-dotted line).

$$H = J \sum_i [(1 + (-1)^i \delta) \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \alpha \mathbf{S}_i \cdot \mathbf{S}_{i+2}], \quad (13)$$

where the  $\mathbf{S}_i$  are again spin- $\frac{1}{2}$  operators at site  $i$ ,  $\alpha$  parametrizes a next-nearest-neighbor coupling, and  $\delta$  is the alternating dimerization.

The two-particle excitations have been discussed in leading order calculations in [17–20]. With our new technique, we perform high-order series expansions in powers of  $\lambda \equiv (1 - \delta)/(1 + \delta)$ . Here we will concentrate only on the expansions for the following two cases:

(1)  $\alpha = 0$ , that is, without the second neighbor interaction. The series for  $\Delta_2$  has been computed up to order 6 for singlet bound states, and to order 11 for triplet and quintet states. Here we find two singlet,  $S_1$  and  $S_2$ , and two triplet,  $T_1$  and  $T_2$ , bound states below the two-particle continuum. The binding energy of these bound states versus momentum  $K$  is given in Fig. 2 for a rather large dimerization  $\delta = 0.6$ . The singlet  $S_1$  exists for the whole range of momenta, while the triplet  $T_1$  exists only in a limited range of momenta, and the singlet  $S_2$  and triplet  $T_2$  bound states occur for momenta in the vicinity of the band maximum at  $K = \pi/2$ . The existence of the second pair of bound states has not been reported by previous calculations, most likely due to a limited precision or a general incapability to deal with multiple bound states. The binding energy at  $K = \pi/2$  versus dimerization  $\delta$  is plotted in Fig. 3. In the limit  $\lambda \rightarrow 0$ , the binding energies for  $S_1$  and  $T_1$  are proportional to  $\lambda$ , as expected, since the formation of these bound states is due to the attraction of two triplets on neighboring sites. For  $S_2$  and  $T_2$ , we find their binding energies are proportional to  $\lambda^2$ . This means that there is a strong enough effective attraction between two triplets separated by a singlet dimer to form those bound states.

(2)  $\alpha = (1 - \delta)/2$ , that is, the expansion is along the disorder line where the ground states are known exactly.

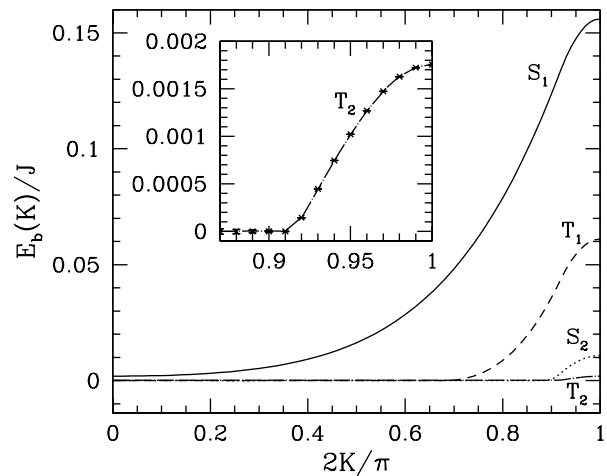


FIG. 2. The binding energy  $E_b$  for two singlet ( $S_1$  and  $S_2$ ) and two triplet ( $T_1$  and  $T_2$ ) bound states versus momentum  $K$  for the  $J_1 - J_2 - \delta$  chain with  $\delta = 0.6$  and  $\alpha = 0$ . The inset enlarges the region near  $K = \pi/2$ .

The series for  $\Delta_2$  has been computed up to order  $\lambda^{19}$  for two-particle singlet, triplet, and quintet states. The two-particle excitation spectrum for  $\delta = 0.4$  is shown in Fig. 4. Here we find that there are three singlet and three triplet bound states below the two-particle continuum, and two quintet antibound states above the continuum. The energy gap at  $K = \pi/2$  for one of the singlet bound states,  $S_1$ , is  $1 + 3\delta$  exactly. In the limit  $\lambda \rightarrow 0$ , the binding energies for  $S_n$  and  $T_n$  ( $n = 1, 2$ ) are of order  $\lambda^n$ , just as for  $\alpha = 0$ , but that for  $S_3$  and  $T_3$  are at most of order  $\lambda^4$ . This calculation demonstrates the power of the method in bringing out the complex character of the pair attraction in the frustrated model.

In conclusion, we have demonstrated a new powerful approach to calculate high-order series expansion for quantum lattice models. The application to the Heisenberg

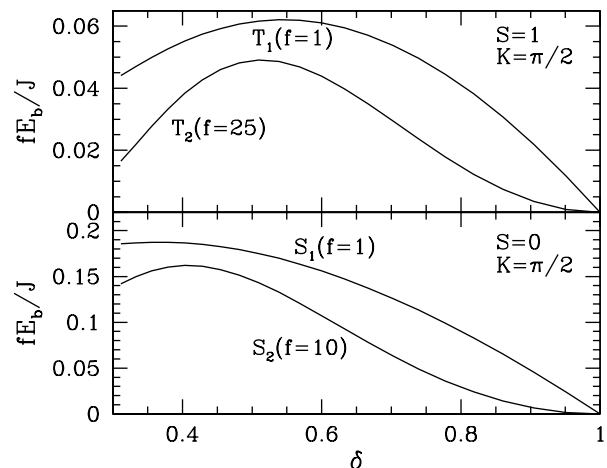


FIG. 3. The scaled binding energy  $fE_b$  at  $K = \pi/2$  versus dimerization  $\delta$  for two singlet ( $S_1$  and  $S_2$ ) and two triplet ( $T_1$  and  $T_2$ ) states of the  $J_1 - J_2 - \delta$  chain with  $\alpha = 0$ , where  $f$  is a scale factor.

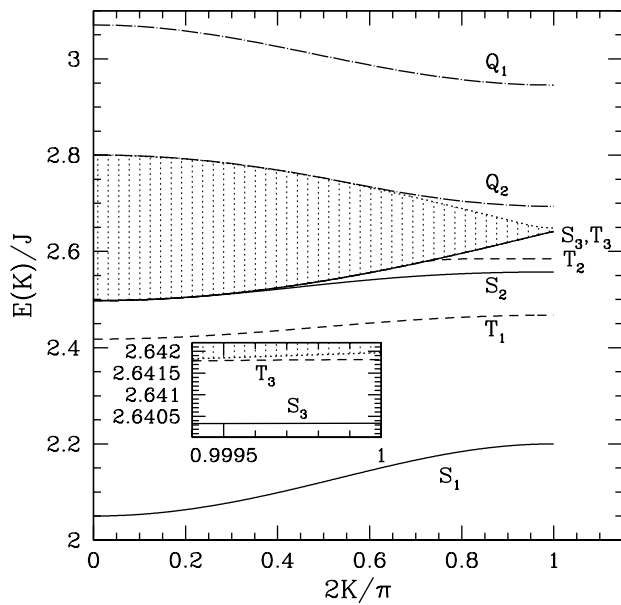


FIG. 4. The excitation spectrum of the  $J_1 - J_2 - \delta$  chain for  $\delta = 0.4$  and  $\alpha = (1 - \delta)/2$ . Beside the two-particle continuum (gray shaded), there are three singlet bound states ( $S_1$ ,  $S_2$ , and  $S_3$ ), three triplet bound states ( $T_1$ ,  $T_2$ , and  $T_3$ ), and two quintet antibound states ( $Q_1$  and  $Q_2$ ). The inset enlarges the region near  $K = \pi/2$  so we can see  $S_3$  and  $T_3$  below the continuum.

spin ladder and the alternating Heisenberg chain yields a precise determination of the low-lying excitation spectra of these models. For the alternating Heisenberg chain it was shown that there are multiple massive singlet and triplet excitations below the continuum, which depend on frustration.

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