

LINKED CLUSTER SERIES EXPANSIONS FOR TWO-PARTICLE STATES IN QUANTUM LATTICE MODELS

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We have developed strong-coupling series expansion methods to study the two-particle spectra in quantum lattice models. The properties of bound states and multiparticle excitations can reveal important information about the dynamics of a given model. At the heart of this method lies the calculation of an effective Hamiltonian in the two-particle subspace. We use an orthogonal transformation to perform this block diagonalising, and find that maintaining orthogonality is crucial for cases where the ground state and the two-particle subspace have identical quantum numbers. The two-particle Schrödinger equation is solved by using a finite lattice approach in coordinate space or an integral equation in momentum space. These methods allow us to determine precisely the low-lying excitation spectra and dispersion relations for the two-particle bound states. The method has been tested for the (1+1) D transverse Ising model, and applied to the two-leg spin-1/2 Heisenberg ladder. We study the coherence lengths of the bound states, and how they merge with the two-particle continuum. Finally, these techniques are applied to the frustrated alternating Heisenberg chain, which has been of considerable recent interest due to its relevance to spin-Peierls systems such as CuGeO_3 . Starting from a limit corresponding to weakly-coupled dimers, we develop high-order series expansions for the effective Hamiltonian in the two-particle subspace. In the regime of strong dimerisation, various properties of the singlet and triplet bound states, and the quintet antibound states, can be accurately calculated. We also study the behaviour as the external bond alternation vanishes, and the way in which the bound states of triplet dimer excitations make the transition to a soliton-antisoliton continuum.

1. The Problem

The study of bound states and multiparticle excitations remains a challenging problem in many-body physics. Experimentally, there are several probes for low-dimensional magnetic or strongly correlated electronic systems which show spectral features associated with multiparticle continuum and bound states. These include

two-magnon Raman spectra, optical absorption, photoemission and neutron scattering spectra. The multiparticle features often remain poorly understood. On the theoretical side, one example of the intriguing issues that may arise is the role that the increasing number of bound states play in the confinement-deconfinement transition in spin-Peierls systems. At the transition the spectrum switches from a soliton-antisoliton continuum to elementary triplet excitations, their bound states and continuum.¹

In this paper, we show how to calculate multi-particle spectral properties from high-order perturbation expansions, using a linked cluster method. A fuller discussion may be found in two recent papers,^{2,3} hereafter referred to as I and II respectively. A brief outline and summary of the work was also given in a recent letter.⁴ Our method is quite distinct from the flow equation approach of Wegner,⁵ which has also been used recently by Uhrig and collaborators^{6,7} for the study of multiparticle spectral properties in one and two dimensions.

2. The Method

We consider a Hamiltonian

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

where the unperturbed Hamiltonian H_0 is exactly solvable, and λ is the perturbation parameter. The aim is to calculate perturbation series in λ for the eigenvalues of H and other quantities of interest. The calculation proceeds in three stages.

2.1. Block diagonalisation

On any finite lattice or cluster of sites, the first step is to ‘block diagonalise’ the Hamiltonian to form an “effective Hamiltonian”, where the ground state sits in a block by itself, the 1-particle states form another block, the 2-particle states another block, and so on. Here a “particle” may refer to a lattice fermion, a spin-flip, or other excitation, depending on the model at hand. We assume that all the unperturbed states in each block are degenerate under H_0 . Here we will only consider the case when the Hamiltonian is real symmetric, and can be block diagonalised by an *orthogonal* transformation,

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

or more conveniently

$$O H^{\text{eff}} = H O, \quad (3)$$

where

$$O^T = O^{-1}. \quad (4)$$

This transformation is constructed order-by-order in perturbation theory. The matrix elements of H^{eff} between different blocks are required to be zero, up to the given order.

The orthogonal transformation will transform the unperturbed two-particle states into “dressed” states containing admixtures of different particle numbers; and in particular, there will be no annihilation process for these “dressed” states. The states will still be labelled by the positions of the original unperturbed particles; but now they will contain admixtures of other particle states at nearby locations.

At any finite order in perturbation theory, we may assume that the effective Hamiltonian will remain “local” (that is, interactions between states will not extend beyond a finite range); and will have the same bulk symmetries as the original Hamiltonian, such as translation symmetry. These properties are sufficient to admit a linked cluster approach to the calculation of eigenvalues.

2.2. Linked cluster expansions

Let us briefly summarise the linked cluster approach in various sectors:

a) Ground-state energy

The ground-state energy E_0 is a simple extensive quantity, and obeys the “cluster addition property”: if C is a cluster (or set of sites and bonds on the lattice) which is composed of two disconnected sub-clusters A and B, then

$$E_0^C = E_0^A + E_0^B . \tag{5}$$

Hence one finds that the ground-state energy per site for the bulk lattice can be expressed purely in terms of contributions from connected sub-clusters α :

$$\epsilon_0 = \sum_{\alpha} l_{\alpha} \epsilon_{\alpha} , \tag{6}$$

where l_{α} is the “lattice constant”, or number of ways per site that cluster α can be embedded in the bulk lattice, and ϵ_{α} is the “proper energy” or “cumulant energy” for the cluster α . In the language of Feynman diagrams, ϵ_{α} can be thought of as the sum of all connected diagrams spanning the cluster α .

A similar formula holds for the ground-state energy of any connected cluster α with open boundaries:

$$E_0^{\alpha} = \sum_{\beta} C_{\beta}^{\alpha} \epsilon_{\beta} , \tag{7}$$

where C_{β}^{α} is the embedding constant of the connected sub-cluster β within cluster α .

Equations (6) and (7) form the basis for a simple and efficient recursive algorithm to generate a perturbation series for ϵ_0 — for further details, see Ref. 1.

b) 1-particle excited states

Gelfand⁸ discovered how to generalise the approach above to one-particle excited states. Let

$$E_1(\mathbf{i}, \mathbf{j}) = \langle \mathbf{j} | H^{\text{eff}} | \mathbf{i} \rangle \tag{8}$$

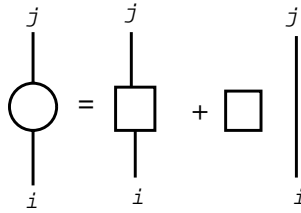


Fig. 1. Decomposition of a 1-particle matrix element into irreducible components. The round box denotes the full matrix element, the square boxes the irreducible matrix elements, and the single line denotes a delta function.

be the matrix element of H^{eff} between initial 1-particle state $|\mathbf{i}\rangle$ and final 1-particle state $|\mathbf{j}\rangle$, labelled according to their positions on the lattice. The excited state energy is not extensive, and does not obey the cluster addition property; but there is a related quantity which does. If cluster C is made up of disconnected sub-clusters A and B, and states $|\mathbf{i}\rangle$ and $|\mathbf{j}\rangle$ reside (say) on cluster A, then

$$E_1^C(\mathbf{i}, \mathbf{j}) = E_1^A(\mathbf{i}, \mathbf{j}) + E_0^B. \tag{9}$$

But if we define the “irreducible” 1-particle matrix element (Fig. 1)

$$\Delta_1(\mathbf{i}, \mathbf{j}) = E_1(\mathbf{i}, \mathbf{j}) - E_0\delta_{\mathbf{i}, \mathbf{j}}, \tag{10}$$

then

$$\Delta_1^C(\mathbf{i}, \mathbf{j}) = \Delta_1^A(\mathbf{i}, \mathbf{j}), \tag{11}$$

whereas if $|\mathbf{i}\rangle$ and $|\mathbf{j}\rangle$ reside on cluster B, then

$$\Delta_1^C(\mathbf{i}, \mathbf{j}) = \Delta_1^B(\mathbf{i}, \mathbf{j}) \tag{12}$$

or in general

$$\Delta_1^C(\mathbf{i}, \mathbf{j}) = \Delta_1^A(\mathbf{i}, \mathbf{j}) + \Delta_1^B(\mathbf{i}, \mathbf{j}), \tag{13}$$

where $\Delta_1(\mathbf{i}, \mathbf{j})$ vanishes for any cluster not containing \mathbf{i} and \mathbf{j} . Note that a 1-particle state cannot annihilate from one sub-cluster and reappear on the other, after the initial block diagonalisation.

From the cluster addition property (13) it follows that the elements $\Delta_1(\mathbf{i}, \mathbf{j})$ can be expanded in terms of contributions from *connected* clusters alone, which are also “rooted”, or connected to the positions \mathbf{i} and \mathbf{j} . Hence they can be calculated efficiently by an algorithm like that for the ground state energy.

c) 2-particle states

The generalisation to two-particle states is now not hard to find. Let

$$E_2(\mathbf{i}, \mathbf{j}; \mathbf{k}, \mathbf{l}) = \langle \mathbf{k}, \mathbf{l} | H^{\text{eff}} | \mathbf{i}, \mathbf{j} \rangle \tag{14}$$

be the matrix element between initial 2-particle state $|\mathbf{i}, \mathbf{j}\rangle$ and final state $|\mathbf{k}, \mathbf{l}\rangle$. To obtain a quantity obeying the cluster addition property, we must subtract the

ground-state energy and 1-particle contributions, to form the irreducible 2-particle matrix element:

$$\begin{aligned} \Delta_2(\mathbf{i}, \mathbf{j}; \mathbf{k}, \mathbf{l}) = & E_2(\mathbf{i}, \mathbf{j}; \mathbf{k}, \mathbf{l}) - E_0(\delta_{\mathbf{i}, \mathbf{k}}\delta_{\mathbf{j}, \mathbf{l}} + \delta_{\mathbf{i}, \mathbf{l}}\delta_{\mathbf{j}, \mathbf{k}}) - \Delta_1(\mathbf{i}, \mathbf{k})\delta_{\mathbf{j}, \mathbf{l}} - \Delta_1(\mathbf{i}, \mathbf{l})\delta_{\mathbf{j}, \mathbf{k}} \\ & - \Delta_1(\mathbf{j}, \mathbf{k})\delta_{\mathbf{i}, \mathbf{l}} - \Delta_1(\mathbf{j}, \mathbf{l})\delta_{\mathbf{i}, \mathbf{k}}. \end{aligned} \quad (15)$$

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. Once again, the block diagonalisation ensures that two particles cannot “annihilate” from one cluster and “reappear” on another disconnected one. Thus the matrix elements of Δ_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} .

2.3. Calculation of eigenvalues

Once the irreducible 1-particle or 2-particle matrix elements are known, they can be inserted into the Schrödinger equation, and then a Fourier transformation will produce a perturbation series expression for the dispersion relation corresponding to the excited states. Some numerical procedures are required to carry through the calculations for the 2-particle states — for details, see Ref. 1.

3. Heisenberg Ladder

The first model we have investigated is the 2-leg spin- $\frac{1}{2}$ Heisenberg ladder, where the Hamiltonian is

$$H = \sum_i \{J_{\perp} \mathbf{S}_i \cdot \mathbf{S}'_i + J[\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \mathbf{S}'_i \cdot \mathbf{S}'_{i+1}]\}, \quad (16)$$

where \mathbf{S}_i (\mathbf{S}'_i) denotes the spin at site i of the first (second) chain. J is the interaction between nearest-neighbour spins along the chain, and J_{\perp} is the interaction between nearest-neighbour spins along the rungs. The antiferromagnetic Heisenberg ladder has attracted a good deal of attention recently. It is of experimental interest in that there are a number of quasi-one-dimensional compounds which may be described by the model.⁹ It is also a prime example of a one-dimensional antiferromagnetic system with a gapped excitation spectrum.

In the dimer limit $J/J_{\perp} = 0$, the ground state is the product state with the spins on each rung forming a spin singlet. The first excited state consists of a spin triplet excitation on one of the rungs.

Here we have calculated series for the dispersions of the 2-particle bound states up to order $(J/J_{\perp})^7$ for the singlet bound state (S), and to order $(J/J_{\perp})^{12}$ for the triplet bound state (T) and the quintet antibound state (Q).

Figures 2 and 3 show the dispersion and the binding/antibinding energy at $J/J_{\perp} = 0.2$ for the two-particle continuum as well as the two-particle bound/antibound states. We can see that there are singlet ($S = 0$) and triplet

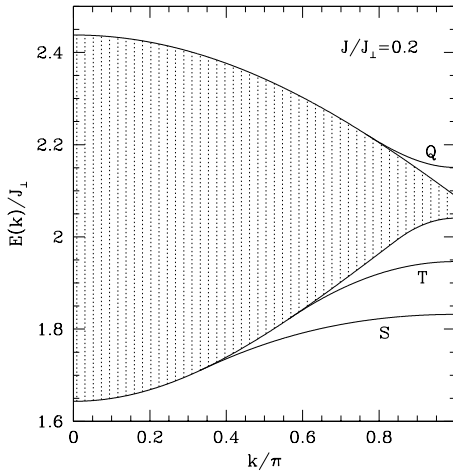


Fig. 2. The excitation spectrum for the Heisenberg spin ladder at $J/J_{\perp} = 0.2$. Beside the two-particle continuum (grey shaded), there are three massive quasiparticles: a singlet bound state (S), a triplet bound state (T) below the continuum and a quintet antibound state (Q) above the continuum.

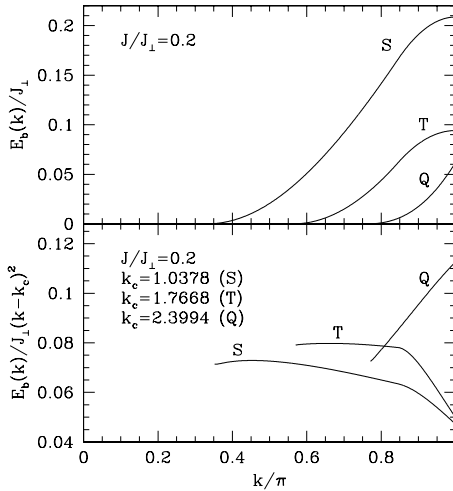


Fig. 3. The binding/antibinding energy E_b/J_{\perp} (upper window) and the rescaled binding/antibinding energy $E_b/J_{\perp}(k - k_c)^2$ (lower window) for the Heisenberg spin ladder at $J/J_{\perp} = 0.2$.

($S = 1$) bound states, made up of two elementary triplets, below the two-particle continuum; and a quintet ($S = 2$) antibound state above the continuum.

From these graphs, we can also see that these bound/antibound states exist only when the momentum k is larger than some “threshold momentum” k_c . We find that the binding energy decreases like $(k - k_c)^2$ as the threshold is approached, at all orders of the expansion, so that this is presumably an exact result.

We have also computed the coherence length L for these bound/antibound states. We find that L diverges like $1/(k - k_c)$ as k approaches k_c , which might be expected since the state becomes unbound at that point. For further details, see Ref. 1.

4. The Frustrated, Alternating Heisenberg Chain

We have also studied the alternating Heisenberg chain with frustration

$$H = \sum_i [(1 + (-1)^i \delta) \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \alpha \mathbf{S}_i \cdot \mathbf{S}_{i+2}], \tag{17}$$

where the \mathbf{S}_i are spin- $\frac{1}{2}$ operators at site i , α parameterises a next-nearest neighbour coupling and δ is the alternating dimerisation. We rewrite the Hamiltonian as

$$H = (1 + \delta) \sum_i [\mathbf{S}_{2i} \cdot \mathbf{S}_{2i+1} + \lambda (\mathbf{S}_{2i} \cdot \mathbf{S}_{2i-1} + y \mathbf{S}_i \cdot \mathbf{S}_{i+2})]. \tag{18}$$

The parameter space (δ, α) is equivalent to the parameter space (λ, y) with $\lambda \equiv (1 - \delta)/(1 + \delta)$ and $y \equiv \alpha/(1 - \delta)$. The latter parametrisation makes explicit that for $\lambda = 0$, the model consists of decoupled dimers: we take this to be our unperturbed Hamiltonian H_0 . The rest of the Hamiltonian can be treated as a perturbation, and we can expand various physical quantities in powers of λ .

This model has been of considerable interest recently because of its relevance to spin-Peierls systems such as CuGeO_3 . The simple spin-1/2 antiferromagnetic chain is well-known to possess fractional ‘spinon’ excitations. The low-lying excitations above the ground-state consist of a two-soliton continuum. Adding a bond-alternation leads to confinement of the spin-half excitations, and the elementary excitations now become triplet states. In the frustrated case, the system is spontaneously dimerised, and there is a gap Δ to the triplet excitations, followed by another gap to the two-triplet continuum at 2Δ . It is interesting to study the transition between the two pictures as the spinons become deconfined.

4.1. Bound states with forced dimerisation; case $\alpha = 0$

First we study the small- λ regime, where our strong coupling expansions are convergent, and a simple truncation of the relevant power series expansions leads to highly accurate results.

We find two singlet (S_1 and S_2) and two triplet (T_1 and T_2) bound states below the two-particle continuum, and two quintet antibound states (Q_1 and Q_2) above the continuum. The two-particle excitation spectrum for a rather large dimerisation $\delta = 0.6$ is shown in Fig. 4. 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 energies and coherence lengths near the threshold momenta behave in the same way as for the previous case of the Heisenberg ladder.

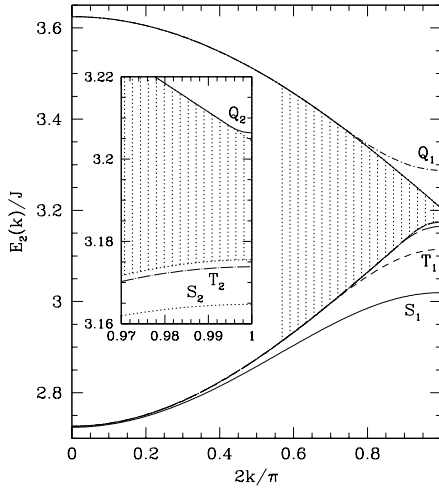


Fig. 4. The excitation spectrum of the $J_1 - J_2 - \delta$ chain with $\delta = 0.6$ and $\alpha = 0$. Beside the two-particle continuum (grey shaded), there are two singlet bound states (S_1 and S_2) and two triplet bound states (T_1 and T_2) below the continuum, and two quintet antibound states (Q_1 and Q_2) above the continuum. The inset enlarges the region near $k = \pi/2$ so we can see S_2 , T_2 and Q_2 below/above the continuum.

4.2. Regime of vanishing bond-alternation: Unbinding of spin-half excitations

Next we turn to the regime of small δ or λ near unity. In this case, our results are less accurate and we have to rely on series extrapolation methods. We use Dlog Padé and integrated differential approximants to extrapolate the series for the single-particle energies and the two-particle binding energies.

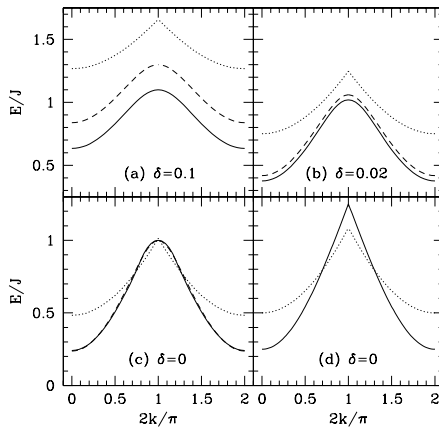


Fig. 5. Dispersion of the single-particle triplet excitation E_1 (solid line), the lowest two-particle singlet bound state S_1 (dashed line), and the bottom of the two-triplet continua (dotted line) for $\delta = 0.1$ (a), 0.02 (b) and 0 (c) for the Shastry-Sutherland model. Window (d) gives the variational results of Shastry and Sutherland, where only the continua are shown.

We study the frustrated model with $\alpha = (1 - \delta)/2$, which is a special line in parameter space where the ground states are known exactly, also known as the Shastry-Sutherland line. The dispersions of the single-particle triplet excitation, the lowest-energy two-particle singlet bound state S_1 , and the bottom of the two-triplet continuum are shown over the full Brillouin zone for various values of δ in Fig. 5. It is evident that the triplet and the singlet spectra become degenerate as δ goes to zero. This is direct evidence for free spin-half excitations, since a pair of free spin-half excitations will form singlet and triplet states of equal energy. Thus the spinons become deconfined as δ goes to zero, as we expect; and it appears that the two-spinon continuum is filled in by a cascade of 2, 3, 4, . . . triplet bound states, in the triplet language, which condense into a continuum in this limit. For further details, see Ref. 2.

5. Conclusions

In conclusion, we have developed new strong-coupling expansion methods to study two-particle spectra of quantum lattice models. We found that one needs to define a two-particle irreducible matrix element, for a cluster expansion to exist. Furthermore, one needs to maintain explicit orthogonality in the transformations in order to study the two-particle subspace characterized by identical quantum numbers to the ground state.

The utility of the method was demonstrated by a detailed study of the properties of 2-particle bound states for the cases of the Heisenberg ladder, and the alternating, frustrated Heisenberg chain.

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