Spectral Weight Contributions of Many-particle Bound States and Continuum

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Cluster expansion methods are developed for calculating the spectral weight contributions of multiparticle excitations - continuum and bound states - to high orders. A complete 11th order calculation is carried out for the alternating Heisenberg chain.

1. Introduction

In recent years there has been a growing interest in understanding quantitatively the single and multiparticle excitation spectra in quantum spin systems. Despite much progress in developing computational methods, the multiparticle excitations remain poorly understood.
Here, we develop a general linked-cluster formalism to calculate the single-particle and multi-particle contributions to the dynamical structure factor by means of high-order series expansions. We apply the method to the alternating Heisenberg chain (AHC) model, where expansions are made around the strong coupling limit of decoupled spin dimers. These structure factors are now amenable to direct experimental measurement, using modern neutron scattering, Raman scattering and other techniques.
The method of linked-cluster series expansions for the calculation of 2-particle energy spectra has been discussed by Trebst et al. [1]. Previous studies of structure factors for 2-particle states include Barnes, Riera and Tennant [2], Tennant et al. [3], who studied the alternating Heisenberg chain; and Knetter, Schmidt, Grüninger and Uhrig [4], who used the method of 'continuous unitary transformations'.

2. Formalism

The inelastic neutron scattering cross section at temperature $T = 0$ is proportional to

$$S^{+-}(k,\omega) = \sum_n S_n^{+-}(k,\omega)$$

where the contribution from intermediate state n is

$$S_n^{+-}(k,\omega) = \delta(\omega - E_n + E_0)\left|\sum_{i^*}\left\langle \Psi_n(k)\middle|S_i^+\middle|\Psi_0\right\rangle e^{ik\cdot r_i}\right|^2$$

and S_i^+ is the spin 'raising' operator at site i. We define

$$S_n^{+-}(k) \equiv N\left|\sum_{i^*}\left\langle \Psi_n(k)\middle|S_i^+\middle|\Psi_0\right\rangle e^{ik\cdot r_i}\right|^2$$

as the "reduced exclusive structure factor" for intermediate state n.

3. Linked Cluster Approach

Matrix elements $S^+(m,i)$ in position space obey a simple linked cluster property:

$$S^+(m,i) = \sum_\gamma s^{\gamma+}(m,i), \qquad \gamma \subset (m,i)$$

where m denotes the position of the dimer excitation, i that of the spin raising operator, and γ denotes a connected or linked cluster of sites on the lattice, which includes both m and i. The algorithm is:

(a) For each cluster γ, calculate the 2-body eigenstates and eigenfunctions following Trebst et al [1];
(b) Calculate matrix elements $S^{+}(m,i)$ for that cluster;
(c) Subtract sub-cluster contributions to get the 'intrinsic' or cumulant contribution of that cluster, and add to the total.

4. Alternating Heisenberg Chain

The Hamiltonian is

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

with the coupling strength alternating between even and odd links. Let

$$H = H_0 + \lambda V$$

where $$H_0 = (1+\delta) \sum_{i \text{ even}} \mathbf{S}_i \cdot \mathbf{S}_{i+1} , \qquad V = \sum_{i \text{ odd}} \mathbf{S}_i \cdot \mathbf{S}_{i+1}$$

and the perturbation parameter is λ = (1-δ)/(1+δ). Then the unperturbed system consists of singlet 'dimer' states on the even links, with the lowest excitation being a triplet excitation on a single link. The alternating chain is thus:

- An isotropic system with a spin gap;
- Possesses S = 1 triplet excitations;
- Possesses 2-particle bound states with S = 0 and 1;
- Has experimental applications, e.g. $Cu(NO_3)_2 2.5 D_2O$ (Xu et al. [5]).

We calculate physical quantities as power series in λ, and the extrapolate to finite λ values using series approximants.

5. Results

Uhrig and Schultz [6] used an RPA approach, and found S = 0 and S = 1 2-particle bound states below the 2-particle continuum. Trebst et al. [1] found that in fact there are *two* S = 0 states and *two* S = 1 bound states below the continuum. We have now calculated structure factors and spectral weights for this system – see the figures, and comments, below.

6. Conclusions

High order series expansions can give detailed and accurate results for structure factors and spectral weights, suitable for comparison with experiment.

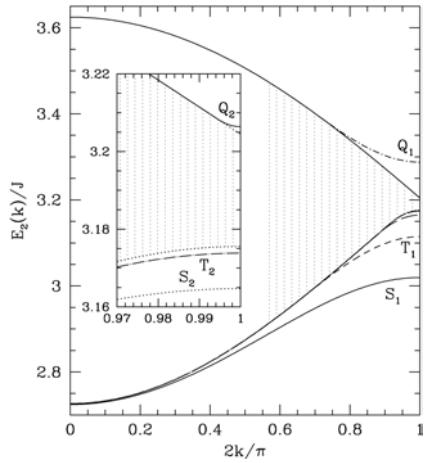

Fig. 1. Dispersion diagram for 2-particle states showing singlet (S) and triplet (T) bound states, plus quintet (Q) 'antibound' states. The inset shows a second pair of bound states below the continuum.

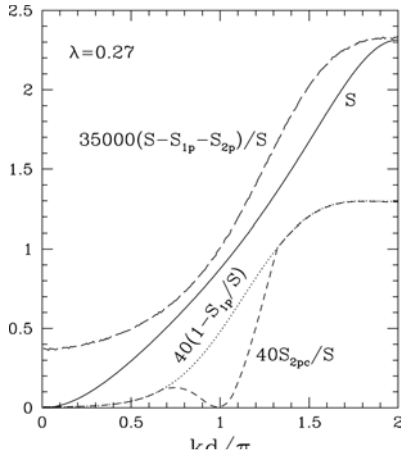

Fig. 2. Structure factors at λ = 0.27, appropriate to the copper nitrate material, as functions of wavevector. S: total; S_{1p}: 1-particle; S_{2p}: 2-particle; S_{2pc}: 2-particle continuum. The 1-particle contributions account for at least 96% of the total.

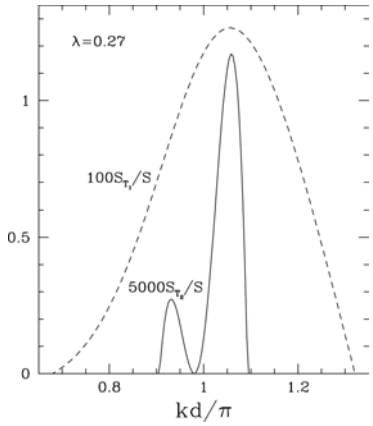

Fig. 3. Relative spectral weights of the triplet bound states T_1 and T_2 at $\lambda = 0.27$. Note the dip in the middle for T_2.

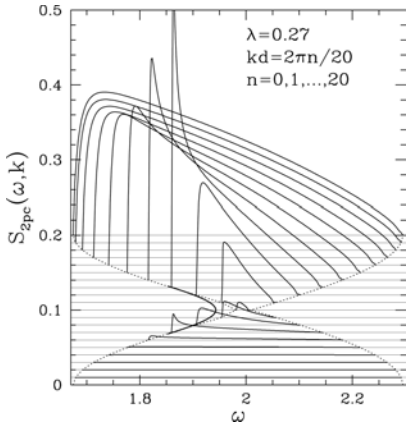

Fig. 4. A 'sliced' view of the structure factor for the 2-particle continuum versus energy for different momenta $kd = 2\pi n/20$, $n = 1,\ldots, 20$ at $\lambda = 0.27$. The solid line is the dispersion relation for the bound state T_1. Note how the structure factor peaks where the bound state enters the continuum.

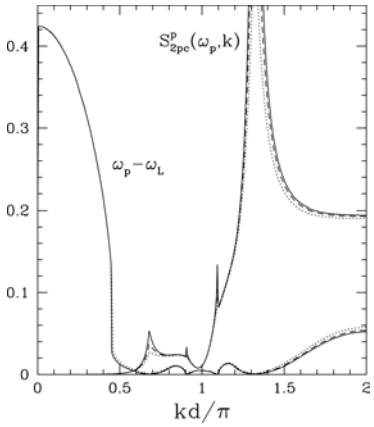

Fig. 5. The peak value of the 2-particle continuum structure factor $S_{2pc}(\omega,k)$, and the difference in energy (ω_p - ω_L) between the position of the peak and the lower edge of the continuum, as functions

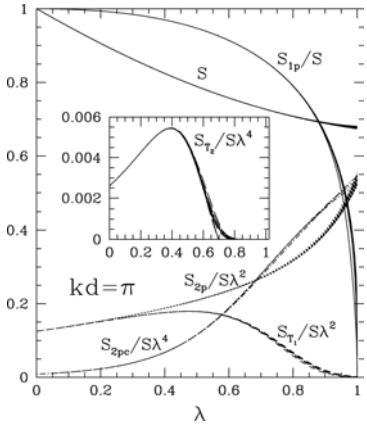

Fig. 6. The relative spectral weights as functions of λ, at $kd = \pi$. Note how the 1-particle spectral weight drops to zero as the uniform limit $\lambda = 1$ is approached; triplet dimer states are no longer relevant for the uniform chain, where the low-energy excitations are 'spinons'.

References

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