Emergence of Composite Spin-one Behaviour in Alternating Spin-1/2 Chains

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We study the alternating antiferromagnetic-ferromagnetic spin-1/2 Heisenberg chain with exchange couplings J and λJ. At small λ the antiferromagnetic bonds form spin-0 dimers, while at large negative λ the ferromagnetic bonds form spin-1 dimers. The crossover is signalled by the merging of the one-particle state with the bottom of the continuum.

1. Introduction

There has been considerable interest recently in the behaviour of the spin excitation spectrum in gapped spin-systems, when a discrete state meets the continuum [1,2]. In one-dimensional systems, the discrete state appears to merge with the bottom of the continuum [3], whereas in higher dimensional systems it appears to enter the continuum in the form of a broadened resonance [4].

Here we apply series expansion methods [5] to the alternating antiferromagnetic-ferromagnetic spin-half Heisenberg chain with Hamiltonian

$$H = \sum_{i} \left[\mathbf{S}_{2i} \, . \, \mathbf{S}_{2i+1} + \lambda \mathbf{S}_{2i-1} \, . \, \mathbf{S}_{2i} \right]$$

This model is particularly interesting in that it interpolates smoothly between the uniform spin-half chain, when $\lambda = 1$, and the limit $\lambda \to -\infty$, when each alternate pair of spins form a spin-1 dimer to minimize the energy, corresponding to a spin-one chain. This model is also interesting from an experimental point of view [6], as several alternating chain compounds are suspected to have an alternating ferromagnetic/antiferromagnetic character.

Our goal here is to study the crossover in the spectrum from the dimerized behaviour near $\lambda = 0$, where the single-particle dominates the spectrum and is well separated from the multi-particle continuum, to the Haldane chain behaviour at large negative λ, where part of the single-particle spectrum begins to overlap with the two-particle continuum.

2. Energy Spectrum

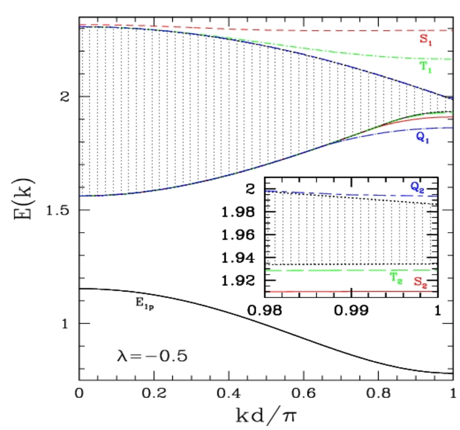

Fig. 1. The spectrum at λ = -0.5. The spacing between dimers is d.

In Fig. 1, we show the single-particle and two-particle spectra calculated for the model at a small coupling λ = -0.5. One can see that the one-particle spectrum E_{1p} has a peak at k = 0 and is well separated from the two-particle continuum (grey shaded). Also shown are the various bound and anti-bound states. The dominant bound and antibound states (S_1, T_1 and Q_1) in the singlet, triplet and quintuplet sectors are reversed with respect to the $\lambda > 0$ case, because the ferromagnetic interaction becomes attractive in the S = 2 channel and repulsive in the S = 0 and S = 1 channels.

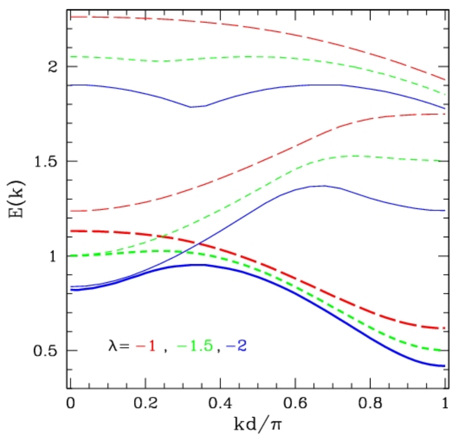

Fig. 2. One particle energies and boundaries of the two-particle continuum at different wavevectors for λ = -1.0 (red curves), -1.5 (green curves) and -2.0 (blue curves).

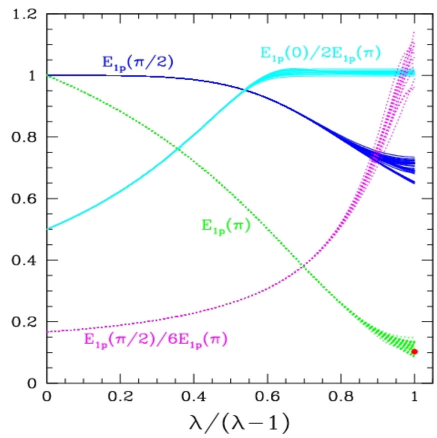

Fig. 3. Single-particle energies and energy ratios at selected wavevectors as a function of λ.

In Fig. 2, we show the one-particle spectra at λ = -1, -1.5 and -2 obtained through series extrapolation methods together with the upper and lower boundaries of the 2-particle continuum. There are several important features to observe here. First, the peak in the single-particle spectrum has moved away from k = 0 and the spectrum is beginning to resemble more the behaviour in Haldane chains. Second, the spectrum near k = 0 potentially overlaps with the two-particle spectrum. We find that the single-particle spectrum rather than moving into the continuum and broadening actually merges with the bottom of the continuum. This is consistent with observations on the Haldane chain materials [3].

Fig. 3 shows a plot of the estimated single-particle excitation energy at momenta kd = $\pi/2$ and kd = π together with the ratio of those energies and the ratio of the excitation energy at k = 0 to that at kd = π, as functions of λ. Values for various integrated differential approximants are shown. The latter ratio saturates at a value of 2 implying again that the one-particle state merges with the bottom of the continuum at k = 0 from this coupling on. It can be seen that $E_{1p}(\pi)$ maps smoothly onto the energy gap for the spin-one chain with an exchange constant of J/4 as $\lambda \to \infty$. The red circle indicates the known gap for the spin-one chain.

3. Structure Factors and Spectral Weights

In Fig. 4, we show the evolution of the integrated structure factor as a function of λ. We see that the crossover to the Haldane chain behaviour is related to the development of a short-range antiferromagnetic peak at kd = π.

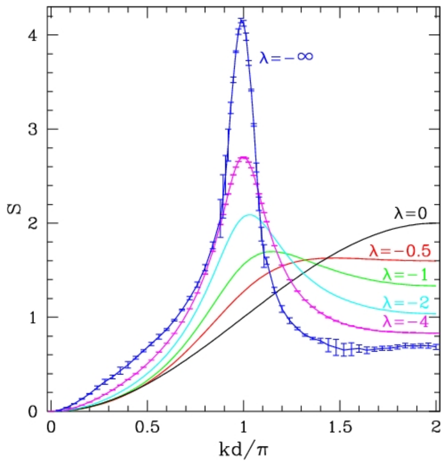

Fig. 4. Evolution of the integrated structure factor S with λ.

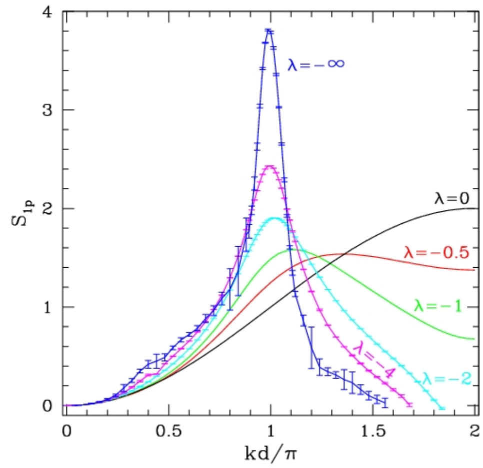

Fig. 5. Single-particle spectral weights (S_{1p}) at different wavevectors as a function of λ.

In Fig. 5, we show the evolution of one-particle spectral weights as a function of λ. We find that in the region where the single-particle spectrum merges with the continuum, its spectral weight becomes very small. Note that the x-axis for this figure runs over $0 < kd < 2\pi$. The spectra are symmetric around $kd = \pi$ and merge with the bottom of the continuum near both $kd = 0$ and $kd = 2\pi$. Near $kd = 0$, the spectral weights are very small to begin with. As the single-particle states merge with the continuum, the weights also become very small near $kd = 2\pi$.

4. Conclusions

We have studied the excitation spectra of the alternating ferromagnetic-antiferromagnetic spin-half chain, and the crossover from the dimerized phase when the antiferromagnetic interactions are stronger to the Haldane phase when the ferromagnetic interactions become stronger. We find that in the former phase the single-particle states are separated from the two-particle continuum and there is a rich spectrum of bound states. In the latter phase the single-particle states are only well defined over part of the Brillouin zone and merge with the bottom of the two-particle continuum near k = 0.

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