Crossover of spectral features from Dimerized to Haldane behavior in alternating antiferromagnetic-ferromagnetic spin-half chains

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We calculate the excitation spectrum and spectral weights of the alternating antiferromagnetic-ferromagnetic spin-half Heisenberg chain with exchange couplings $J$ and $-|\lambda|J$ as a power series in $\lambda$. For small $|\lambda|$, the gapped one-particle spectrum has a maximum at $k = 0$ and there is a rich structure of bound (and anti-bound) states below (and above) the 2-particle continuum. As $|\lambda|$ is increased past unity the spectrum crosses over to the Haldane regime, where the peak shifts away from $k = 0$, and the spectral weights associated with the one-particle states become very small. Extrapolation of the spectrum to large $|\lambda|$ confirms that the ground state energy and excitation gap map onto those of the spin-one chain.

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Recently there has been considerable interest in termination of the spin excitation spectrum in gapped spin systems, when a discrete state meets the continuum. This issue has been studied theoretically\textsuperscript{1,2} and experimentally in one\textsuperscript{3,4,5} and higher dimensional\textsuperscript{6} systems. One interesting observation is that while in the one-dimensional case the spectrum appears to merge with the bottom of the continuum,\textsuperscript{3} in the higher dimensional system it appears to enter the continuum in the form of a broadened resonance.\textsuperscript{6}

Controlled and systematic numerical calculation of the spin dynamics of quantum spin models remains a challenging computational task.\textsuperscript{7} Despite much progress in developing computational methods there are few methods that can accurately calculate even the single-particle spectrum. Calculations of the multi-particle continuum and bound states remains even more daunting, with series expansion methods clearly leading the way.\textsuperscript{8,9,10,11}

We have recently developed a linked-cluster formalism to calculate the single-particle and multi-particle spectra and spectral weights of quantum spin models by means of high-order series expansions.\textsuperscript{12,13,14} Here, we apply the method to the alternating antiferromagnetic-ferromagnetic spin-half Heisenberg chain with Hamiltonian

$$H = \sum_i \left[ S_{2i} \cdot S_{2i+1} + \lambda S_{2i-1} \cdot S_{2i} \right] \quad (1)$$

This model is particularly interesting in that it interpolates smoothly between the spin-half chain ($\lambda \rightarrow 1$) and the spin-one chain ($\lambda \rightarrow -\infty$). The case of positive $\lambda$ corresponds to the antiferromagnetic alternating Heisenberg chain (AHC) and has been studied extensively in the literature.\textsuperscript{15} Our goal here is to study the negative $\lambda$ model. In particular we are interested in the crossover in the spectrum from the dimerized behavior near $\lambda = 0$, where the single-particle dominates the spectrum and is well separated from the multi-particle continuum, to the Haldane chain behavior at large $|\lambda|$, where part of the single-particle spectrum begins to overlap with the two-particle continuum. One of the interesting questions is, what happens to the single-particle spectrum and spectral weights as the single-particle states meet the two-particle continuum? Here we use the same notation as in reference 13.

We also present quantitative studies of bound and anti-bound states in the model. The latter can only be done reliably when $|\lambda|$ is not too large, as it is unclear how series extrapolation methods can be applied to the multi-particle spectra. We find that there are two bound/antibound states in each of the $S = 0$, $S = 1$ and $S = 2$ sectors, of which a bound state in each sector disappears between $-1 > \lambda > -2$. We also extrapolate the ground state energy and the spin-gap at $k = \pi$ to $\lambda \rightarrow -\infty$ to confirm the mapping of the model to the spin-one Heisenberg chain.\textsuperscript{15}

This model is also interesting from an experimental point of view,\textsuperscript{16} as several alternating chains are suspected to have an alternating ferromagnetic/antiferromagnetic character. One of our motivations is to present detailed results on spectral weights for bound states and multi-particle continua which can help the search for these features in experiments.

Throughout this paper we assume the inter-dimer spacing is $d$ and that all spins are equally spaced at a distance $d/2$. We have calculated the spectrum for a more general geometry, where the dimers are oriented in some way with respect to the chain, and where the projected distance between neighboring spins within the dimer and between dimers may be different.\textsuperscript{17} These are likely very important for a detailed comparison with specific experimental systems but not important for discussing the gen-
eral properties. These series, or the extrapolated plots can be obtained from the authors on request.

We begin with a discussion of the spectrum for small $|\lambda|$, where no series extrapolation is needed and simple summation leads to very accurate results. In Fig. 1, we show the single-particle and two-particle spectra calculated for the model at $\lambda = -0.5$. One can see that the one-particle spectrum has a peak at $k = 0$ and it is well separated from the two-particle continuum. Also shown are the various bound and anti-bound states. It is not difficult to understand why 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. The ferromagnetic interaction becomes attractive in the $S = 2$ channel and repulsive in the $S = 0$ and $S = 1$ channels. The behavior of the weaker bound and antibond states ($S_2, T_2$ and $Q_2$) arises from further neighbor interactions generated in higher orders of perturbation theory. Hence, they are harder to treat analytically.

In Fig. 2 we show the spectral weights associated with the various states. It is evident that the one particle state carries the most weight. For $kd < \pi$ almost all the weight lies in the single-particle spectrum. The two-particle weights peak at $kd = 2\pi$. In Fig. 3 the relative contributions for one and two-particle states are shown. At $kd = 2\pi$ the two-particle weights can reach above 13 percent. The sum of one and two-particle weights for all $k$ carries about 99.9 percent of the weight. Thus, there is negligible spectral weight in states with more than two particles. In Fig. 4 the relative weight in the two bound states is shown as a function of $k$. Note that the anti-bound state $T_1$, lying above the continuum, still carries the dominant weight. Both weights remain small at all $k$ and thus may not be easy to observe experimentally, the largest weight fraction being less than 4 percent.

To see the evolution of the model as $|\lambda|$ is increased past unity, we need to use series extrapolation methods. In Fig. 5, we show the evolution of the integrated structure factor as a function of $|\lambda|$. We see that the crossover
to the Haldane chain behavior is related to the development of a short-range antiferromagnetic peak at \( kd = \pi \).

Our results at \( \lambda = -\infty \) agree with an extrapolation of the finite lattice results of Takahashi\(^{20}\) for the spin-1 chain at \( k = \pi \).

In Fig. 6, we show the spectrum at \( \lambda = -1, -1.5 \) 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 behavior 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. 4: Relative weights of bound state \((T_2)\) and antibound state \((T_1)\) at different wavevectors for \( \lambda = -0.5 \).

FIG. 5: (Color online) Evolution of the integrated structure factor \( S \) with \(|\lambda|\). The red point is an extrapolation of the finite lattice results of Takahashi\(^{20}\) at \( k = \pi \).

FIG. 6: (Color online) One particle energies (solid curves) and upper and lower boundaries of the two-particle continuum (dashed curves) at different wavevectors for \( \lambda = -1.0 \) (red curves), \(-1.5\) (green curves) and \(-2.0\) (blue curves).

FIG. 7: (Color online) Single-particle spectral weights \((S_{1p})\) at different wavevectors as a function of \( \lambda \).

In Fig. 7, we show the evolution of one-particle spectral weights as a function of \( \lambda \). 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 $kd = 2\pi$.

Extrapolating the full spectrum to larger $|\lambda|$ proves difficult. The spectrum at small $k$ shows poor convergence, which may be related to the fact that single-particle states are not well defined at small $k$, and the spectrum is not a monotonically decreasing function of $\lambda$. However, extrapolating the ground state energy, and the single-particle excitation energy in the range $\pi/2 < kd < \pi$, we have verified that the model maps on to the spin-one chain with an exchange constant of $J/4$, with numerical values in agreement with DMRG studies on the spin-one chain. Fig. 8 shows a plot of the estimated single-particle excitation energy at momenta $kd = \pi/2$ and $kd = \pi$ together with the ratio of those energies and the ratio of the excitation energy at $k = 0$ to that at $kd = \pi$, as functions of $\lambda$. 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 as $\lambda \to -\infty$.

In conclusion, in this paper 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 $k = 0$. We present detailed results for various spectral weights, including bound states and continua, which can be helpful in experimental searches for these subtle effects.

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