Structure Factors and Multi-Particle Dynamics From Series Expansions

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We develop a linked cluster method to calculate the spectral weights of many-particle excitations at zero temperature, and apply these methods to the alternating Heisenberg chain. In agreement with Schmidt and Uhrig [1], we find that the spectral weight is dominated by 2-triplet states, even at $\lambda = 1$.

1. Introduction

Powerful new facilities for neutron scattering and Raman scattering experiments are beginning to explore the detailed multi-particle dynamics of condensed matter systems. A probe such as an incoming neutron scatters from the system, delivering energy and momentum and forming an excited state of the system (Fig. 1).

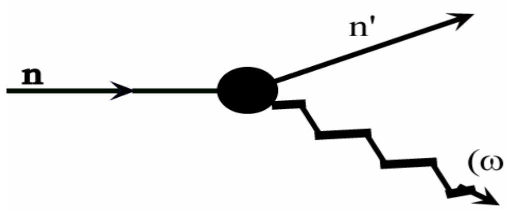

Fig. 1

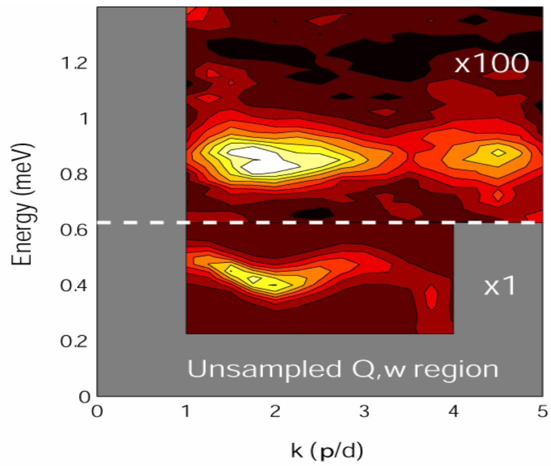

Fig. 2

The scattering probability is proportional to the *structure factor* for the system. Figure 2 is an example of experimental data [2] for the material $Cu(NO_3)_2.2.5D_2O$, showing one-magnon and two-magnon contributions to the structure factor. We have been developing series expansion methods to calculate dispersion relations and structure factors for quantum lattice models at zero-temperature. We split the Hamiltonian into two parts:

$$H = H_0 + \lambda H_1$$

where H_0 is a soluble term which can be exactly diagonalized, H_1 is treated as a perturbation, and physical quantities are expressed as high-order power series in λ. The parameter λ can then be set to its physical value. Our group has developed sophisticated linked-cluster methods for performing these calculations [3,4,5].

2. Example: The Alternating, Frustrated Heisenberg Chain (AHC)

$$H = \Sigma \{[1+(-1)^i\delta]S_i.S_{i+1} + \alpha S_i.S_{i+2}\}$$

This is a relatively simple 1-dimensional model [Fig.3(a)] with interesting dynamics; the material $Cu(NO_3)_2.2.5D_2O$ is thought to be an experimental realization. Define parameters $\lambda = (1-\delta)/(1+\delta)$, $y = \alpha/(1-\delta)$, then

$$H = (1+\delta)\sum_i [S_{2i}.S_{2i+1} + \lambda(S_{2i-1}.S_{2i} + yS_i.S_{i+2})] .$$

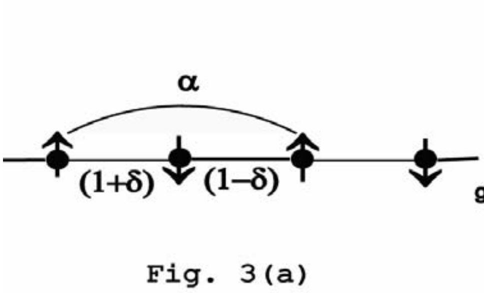

Fig. 3(a)

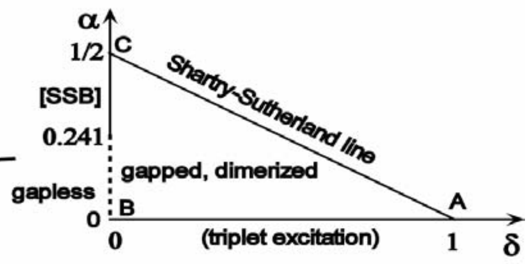

Fig. 3(b)

Phase Diagram: Fig. 3(b)

Point A: Fully dimerized ground state with each pair of sites forming a spin-singlet *dimer*. Excited states are S=1 triplet excitations on each dimer, with an energy gap.
Point B: Uniform Heisenberg chain (with $\alpha = 0$). The energy gap is zero; the system is described in term of spin-1/2 *spinon* excitations. As $\delta \to 0$, the gap vanishes as
$\Delta(\delta) \sim \delta^{2/3}/\sqrt{\ln(\delta/\delta_0)}$
Point C: The Majumdar-Ghosh point. The dimerized ground state is an exact eigenstate along the Shastry-Sutherland line; the system remains dimerized, and gapped. At $\delta = 0$, spontaneous symmetry breaking produces a gap beyond the critical value $\alpha_c \sim 0.241$ of the frustration parameter.

Field theory predicts just *two* bound states of triplets (S=1 and S=0) at the critical point, with mass ratio $\sqrt{3}$ between them.

At C, excitations are again *spinons*. For small δ, spinons are *confined* by a linear potential, and the low-lying spectrum is discrete. As $\delta \to 0$, the spectrum becomes continuous.

3. Results

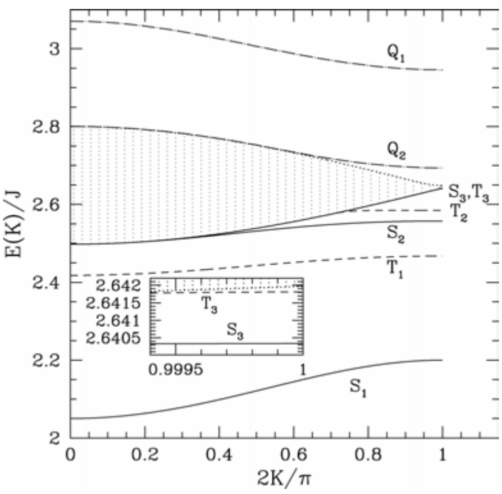

Figure 4: Spectrum of 2-triplet states at $\delta = 0.4$, on the Shastry-Sutherland line. Note the appearance of multiple S=0 and S=1 bound states (S and T respectively), and S=2 anti-bound states (Q).

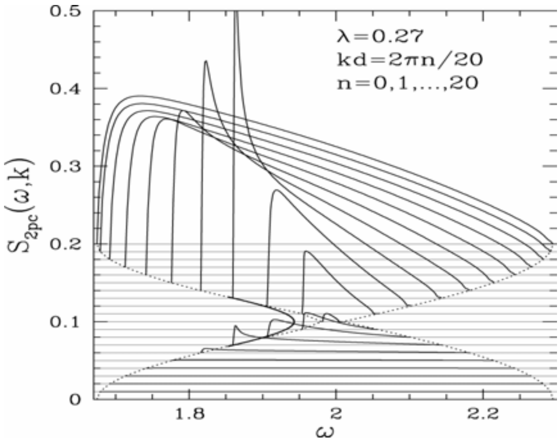

Figure 5: Calculated structure factor at $\lambda = 0.27$ as function of energy ω, for various momentum slices. The solid line marks the dispersion relation of the T_1 bound state. Note the sharp spikes developing where the bound-state enters the continuum.

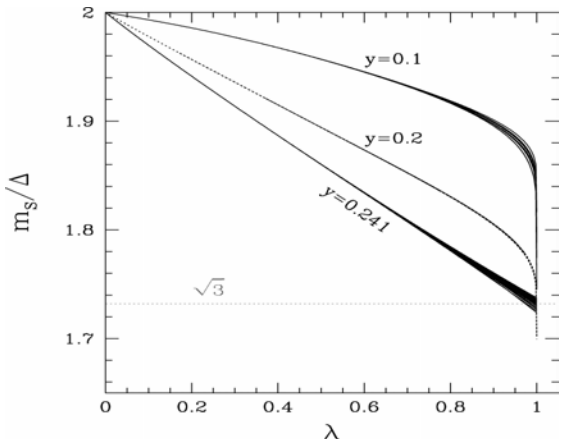

Figure 6: Our estimates of the mass ratio as function of λ, for various y values. Note the sharp (logarithmic?) downturn towards $\sqrt{3}$ near $\lambda = 1$.

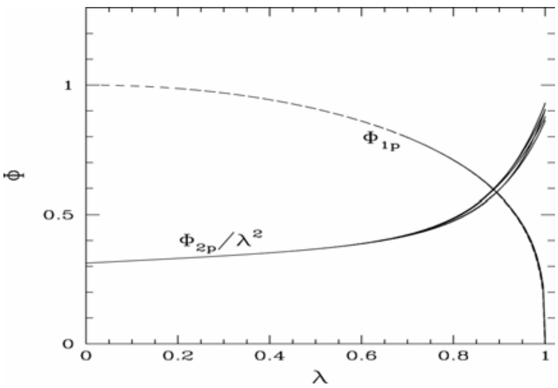

Figure 7: Integrated contributions to the structure factor. As $\lambda \to 1$, the 1-particle contribution goes to zero, while the 2-particle contribution increases to near 100%. This indicates a *triplet* description should be equally valid with a *spinon* description.

4. Questions

Is the mass ratio equal to $\sqrt{3}$ for all $\alpha < \alpha_c$ at $\delta = 0$?
How does the *triplet* description cross over to a *spinon* description as $\delta \to 0$?
How do discrete triplet excitations form a *continuous* spinon-antispinon spectrum as $\delta \to 0$ for $\alpha > \alpha_c$?

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References

[1] K.P. Schmidt and G.S. Uhrig, Phys. Rev. Lett. 90, 227204 (2003)
[2] D.A. Tennant *et al.*, Phys. Rev. B67, 054414 (2003).
[3] S. Trebst, H. Monien, C.J. Hamer, W. Zheng, R.R.P. Singh, Phys. Rev. Lett. 85, 4373 (2000).
[4] W. Zheng, C.J. Hamer, R.R.P. Singh, S. Trebst, H. Monien, Phys. Rev. B63, 144411 (2001).
[5] C.J. Hamer, W. Zheng, R.R.P. Singh, Phys. Rev. B68, 214408 (2003).