Topic area: **CMMSP**

Magnon Dispersion and Structure Factors for Heisenberg Antiferromagnets

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The building of new and more powerful neutron scattering facilities is allowing a more detailed exploration of the dynamical properties of condensed matter systems, including the dispersion relations and structure factors of the low-lying quasiparticle excitations. Here we set out to compute the properties of single magnon states in the Heisenberg model of an antiferromagnet on the square and cubic lattices, using high-order series expansions [1].

The Hamiltonian for the spin-$\frac{1}{2}$ anisotropic Heisenberg antiferromagnet is

$$H = J \sum_{\langle ij \rangle} [S_i^z S_j^z + x(S_i^x S_j^x + S_i^y S_j^y)] \ , \tag{1}$$

where the sum runs over nearest-neighbor pairs of sites. The limits $x = 0$ and $x = 1$ correspond to the antiferromagnetic Ising model and isotropic Heisenberg model, respectively. The first term is taken as the unperturbed Hamiltonian, with the unperturbed ground state being the usual Neél state. The second term is treated as a perturbation. It flips a pair of spins on neighbouring sites.

The Ising series for ground state properties has been computed before [2]. Here we compute the series for the 1 magnon dispersion up to order x^{14} for the square lattice, and to order x^{10} for the simple cubic lattice. We also compute the integrated structure factor for this system [3]. Depending on the neutron scattering beam, one can define the following 3 different integrated structure factors: the integrated unpolarized structure factor $S_{\rm xyz}(\mathbf{k})$, the integrated longitudinal structure factor $S_{\rm zz}(\mathbf{k})$ and also the integrated transverse structure factor $S_{\rm xy}(\mathbf{k})$

$$S_{\rm xyz}(\mathbf{k}) = \frac{1}{N} \sum_{ij} e^{i\mathbf{k}\cdot(\mathbf{r}_j - \mathbf{r}_i)} \left(\langle S_i^z S_j^z + S_i^x S_j^x + S_i^y S_j^y \rangle_0 - \langle S_i^z \rangle_0 \langle S_j^z \rangle_0 \right) \tag{2}$$

$$S_{\rm zz}(\mathbf{k}) = \frac{1}{N} \sum_{ij} e^{i\mathbf{k}\cdot(\mathbf{r}_j - \mathbf{r}_i)} \left(\langle S_i^z S_j^z \rangle_0 - \langle S_i^z \rangle_0 \langle S_j^z \rangle_0 \right) \tag{3}$$

$$S_{\rm xy}(\mathbf{k}) = \frac{1}{N} \sum_{ij} e^{i\mathbf{k}\cdot(\mathbf{r}_j - \mathbf{r}_i)} \langle S_i^x S_j^x + S_i^y S_j^y \rangle_0 \ , \tag{4}$$

where $\langle \cdots \rangle_0 = \langle \psi_0 | \cdots | \psi_0 \rangle$ denotes the ground state expectation value. To make the series expansion much more efficient, we have subtracted in $S_{\rm zz}(\mathbf{k})$ and $S_{\rm xyz}(\mathbf{k})$ the term

$$\frac{1}{N} \sum_{ij} e^{i\mathbf{k}\cdot(\mathbf{r}_j - \mathbf{r}_i)} \langle S_i^z \rangle_0 \langle S_j^z \rangle_0 \ . \tag{5}$$

It can easily be proven that this term gives a δ-function, with the peak at $\mathbf{k} = (\pi, \pi)$ corresponding to antiferromagnetic order.

We also compute the structure factor for the 1-magnon state, which can only couple with the ground state via the transverse terms in H, defined as

$$S_{1\mathrm{p}}(\mathbf{k}) = \frac{1}{N}\sum_{ij} e^{i\mathbf{k}\cdot(\mathbf{r}_j-\mathbf{r}_i)}(\langle\psi_0|S_i^x|\psi_1\rangle\langle\psi_1|S_j^x|\psi_0\rangle + \langle\psi_0|S_i^y|\psi_1\rangle\langle\psi_1|S_j^y|\psi_0\rangle) . \quad (6)$$

The series for these quantities have been computed up to order x^{14} for the square lattice, and to order x^{10} for the simple cubic lattice. The calculations involve a list of 4654283 clusters, up to 15 sites for the square lattice, and 1487597 clusters, up to 11 sites for the simple cubic lattice.

With this, we can compute the multiple-magnon spectral weight contribution to neutron scattering

$$W_{\mathrm{xy}}(\mathbf{k}) = 1 - S_{1\mathrm{p}}(\mathbf{k})/S_{\mathrm{xy}}(\mathbf{k}) \quad (7)$$

$$W_{\mathrm{xyz}}(\mathbf{k}) = 1 - S_{1\mathrm{p}}(\mathbf{k})/S_{\mathrm{xyz}}(\mathbf{k}) , \quad (8)$$

where W_{xy} is the multiple-magnon contribution to polarized neutron scattering, while W_{xyz} is the multiple-magnon contribution to unpolarized neutron scattering.

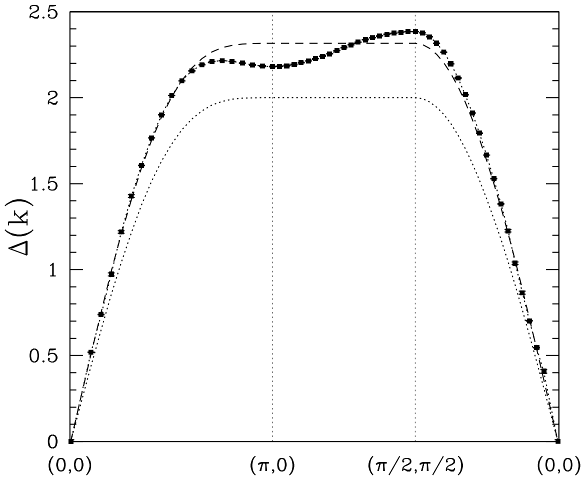

Figure 1: The 1-magnon excitation spectrum $\Delta(k_x, k_y)$ along high-symmetry cuts through the Brillouin zone for the Heisenberg antiferromagnet on a square lattice. Also shown are the results of first order (dotted line) and second order (dashed line) spin-wave theory.

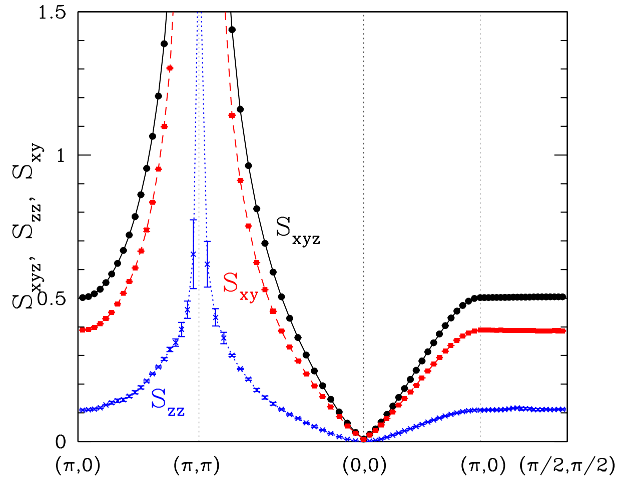

Figure 2: The various integrated structure factor S_{xyz} (unpolarized) , S_{xy} (transverse) and S_{zz} (longitudinal) along high-symmetry cuts through the Brillouin zone for the Heisenberg antiferromagnet on a square lattice.

We compare our results for the one-magnon dispersion with spin-wave theory. The second order spin-wave theory [2] predicts the 1-magnon dispersion as

$$\Delta(\mathbf{k}) = zS(1 - C_1/(2S))(1-\gamma_k^2)^{1/2} , \quad (9)$$

where z is the coordination number of the lattice, γ_k is the structure factor of the lattice

$$\gamma_k = \frac{1}{z}\sum_{\rho} e^{i\mathbf{k}\cdot\rho} \quad (10)$$

and C_1 is defined by

$$C_1 = \frac{2}{N}\sum_k [(1-\gamma_k^2)^{n/2} - 1] \tag{11}$$

which is -0.157947 for the square lattice, or -0.097158 for the simple cubic lattice.

Figure 1 shows the 1-magnon excitation spectrum $\Delta(k_x, k_y)$ along high-symmetry cuts through the Brillouin zone for the Heisenberg antiferromagnet on a square lattice, together with the results of first and second order spin-wave theory. We can see that the dispersion is gapless at $(0,0)$ or the equivalent point (π,π), which of course reflects the Goldstone nature of the magnon excitations, and the spin-wave theory predicts a flat dispersion from $(\pi,0)$ to $(\pi/2,\pi/2)$, while the series gives the excitation energy at $(\pi/2,\pi/2)$ about 9.3% higher than that at $(\pi,0)$. This is in agreement with experimental data for $Cu(DCOO)_2 \cdot 4D_2O$ (CFTD) [4] and $Sr_2Cu_3O_4Cl_2$ [5], but opposite to La_2CuO_4. [6]

Figure 2 shows various integrated structure factors S_{xyz} (unpolarized) , S_{xy} (transverse) and S_{zz} (longitudinal). We can see that they are zero at the $(0,0)$ point, and diverge at the (π,π) point. We can also see that S_{xy} is more than twice the size of S_{zz}, reflecting that the system is in an ordered phase.

The 1-magnon structure factor S_{1p}, together with the multiple-magnon spectral weights W_{xy} and W_{xyz}, are shown in Figure 3. We can see that S_{1p} is zero at the $(0,0)$ point and diverges at the (π,π) point, and the maximum multiple-magnon contribution in polarized (unpolarized) neutron scattering is about 26.8% (34.7%) at the $(\pi,0)$ point.

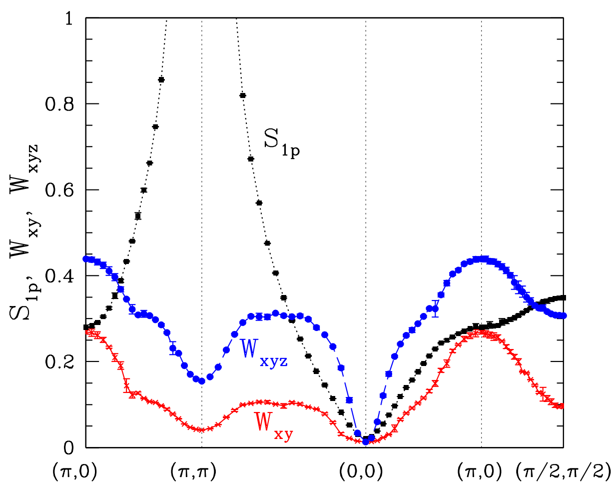

Figure 3: The 1-magnon structure factor S_{1p}, and various multi-magnon spectral weights W_{xy} and W_{xyz} for the Heisenberg antiferromagnet on a square lattice.

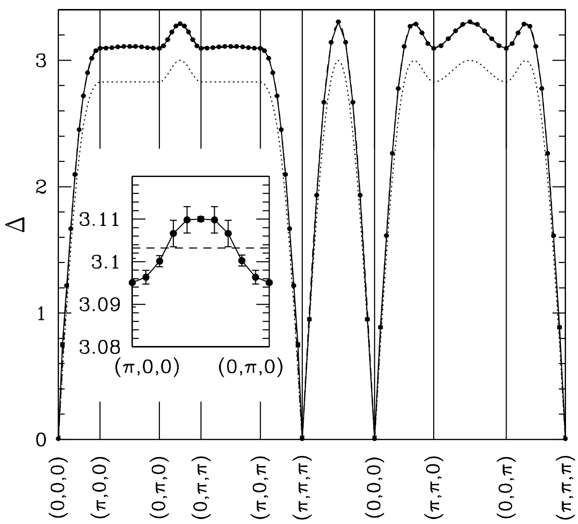

Figure 4: The 1-magnon excitation spectrum $\Delta(k_x, k_y)$ along high-symmetry cuts through the Brillouin zone for the Heisenberg antiferromagnet on a simple cubic lattice. Also shown are the results of first order (dotted line) and second order (dashed line) spin-wave theory.

Similar results for the simple cubic lattice are presented in Figures 4-6. We can see that for the dispersion, the second order spin-wave theory gives almost the same results as the series: the difference only becomes visible when we enlarge the figures, as shown in the insert, where the spin-wave theory shows a flat dispersion between $(\pi,0,0)$ and $(0,\pi,0)$, while the series gives a small peak in the middle. Figure 6 also shows that the maximum multiple-magnon contribution in polarized (unpolarized) neutron scattering is about 3% (15.5%), much smaller than for the square lattice.

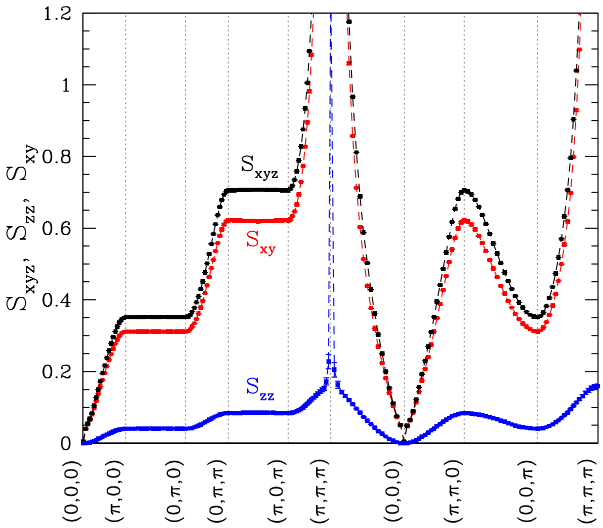

Figure 5: The various integrated structure factor S_{xyz} (unpolarized) , S_{xy} (transverse) and S_{zz} (longitudinal) along high-symmetry cuts through the Brillouin zone for the Heisenberg antiferromagnet on a simple cubic lattice.

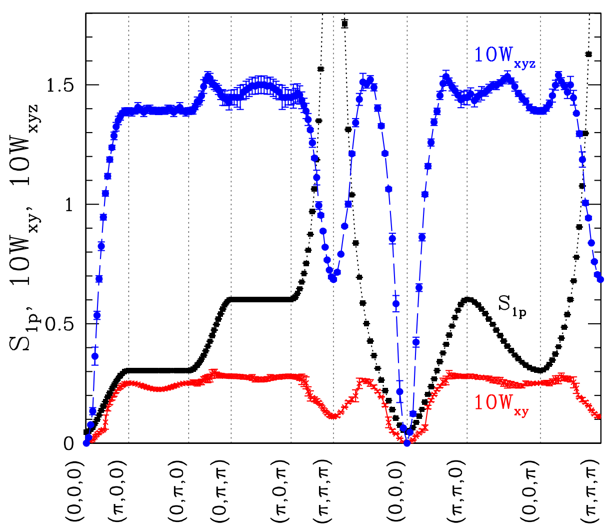

Figure 6: The 1-magnon structure factor S_{1p}, and various multi-magnon spectral weights W_{xy} and W_{xyz} for the Heisenberg antiferromagnet on a simple cubic lattice.

In conclusion, it can be seen that for the simple cubic lattice there is almost perfect agreement between the series extrapolation results and the predictions of second-order spin-wave theory for the single magnon dispersion relation. For the square lattice, the agreement is not quite so spectacular, but is still very good for low momenta. It would be very interesting to see if similar agreement is found for the structure factors – the spin-wave theory has not been taken to second order for these quantities, as far as we aware. It would also be interesting to see how the results compare with experimental measurements.

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