Multispinon Continua at Zero and Finite Temperature in a Near-Ideal Heisenberg Chain

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SUPPLEMENTAL MATERIAL - MULTISPINON CONTINUA AT ZERO AND FINITE TEMPERATURE IN A NEAR-IDEAL HEISENBERG CHAIN

EXPERIMENTAL DETAILS

The $KCuF_3$ sample was a single crystal with a mass of 6.86 g. The neutron scattering data were collected using the MAPS time-of-flight spectrometer at the ISIS pulsed neutron spallation source in the Rutherford Appleton Laboratory, U.K. The crystal was aligned with the chains (c-axis) horizontal and perpendicular to the incident neutron beam while the a-axis was parallel to the incident beam. A Fermi chopper was phased to select neutrons with a fixed incident energy of 150 meV and a chopper frequency of 500 Hz was chosen to yield an energy resolution of 4.9, 3.7 and 2.6 meV at energy transfers of 0, 50, 120 meV respectively. The sample was cooled in a closed cycle cryostat and data were collected at temperatures of 6, 50, 75, 150, 200, 300 K. Counting times were typically between 700 and 3800 μAmp (4-22 hours). The datasets consisted of the neutron counts collected in the large position sensitive detector array as a function of their time of arrival.

DATA TREATMENT

The data were corrected for detector efficiency and normalized to absolute units using white and monochromatic neutron scattering measurements of a standard Vanadium sample along with the known mass of the $KCuF_3$ sample. The data were then converted to energy transfer ($\hbar\omega$) and wavevector transfer along all three reciprocal lattice directions of $KCuF_3$ ($\boldsymbol{k} = (k_a, k_b, k_c)$) using standard software available at ISIS. The energy transfers were given by the incident neutron energy minus the final neutron energies (calculated from the times the neutrons took to reach the detector); the conversion to wavevector transfer was performed by taking into account the orientation of the sample and the positions on the detector of the scattered neutrons as well as the incident and final neutron energies. Each dataset then consisted of many thousands of pixels each giving the signal at different energy and wavevector transfers labeled by $(k_a, k_b, k_c, \hbar\omega)$. Finally the background was modelled by extrapolating the signal measured in regions where the dynamical structure factor is known to be (approximately) zero e.g. at $k_c = 0, 2\pi$, all $\hbar\omega$ and $k_c = \pi/2$, $\hbar\omega < \pi J/2$; this was then subtracted from the data to obtain the magnetic signal. The different cuts and slices through the data shown in the figures were performed using the MSLICE program where in all cases the data were integrated over directions perpendicular to the chain (i.e. over k_a and k_b).

COMPARISON TO THEORETICAL RESULTS

In order to compare the various theories of the spin-1/2 Heisenberg antiferromagnetic chain with the experimental data, we simulated the scattering that would be expected experimentally for each theory. This was achieved by calculating the theoretical $S(k_c, \omega)$ for all the different $(k_a, k_b, k_c, \hbar\omega)$ that make up the experimental datasets. Since $S(k_c, \omega)$ is one-dimensional the components of wavevector transfer perpendicular to the chain (k_a and k_b) were ignored. Before this could be done however a number of corrections were applied to the theoretical $S(k_c, \omega)$. First of all it was multiplied by the square of the anisotropic copper form factor $F_{Cu}(k_a, k_b, k_c)$, secondly in order to model the instrumental resolution, it was convolved numerically by a Gaussian whose width was the energy-dependent resolution obtained from the MCHOP program. The simulations also took into account the mosaic spread of the sample. This was achieved by performing a series of simulations that stepped through the known angular width of the sample, these were then added and normalised.

The resulting simulated datasets were identical in form to the experiment datasets and all manipulations performed on the real data were also performed on the virtual data (except background subtraction and normalization). Direct comparison between theory and experiment was achieved by using the MSLICE program to perform the same cuts and slices on the virtual and real datasets (see figures). Finally it should be noted that because the data were in absolute units no additional overall factor was included in the simulations when making these comparisions.