Density Matrix Renormalization Group Method Enables Computing High-Resolution Magnetic Excitation Spectra

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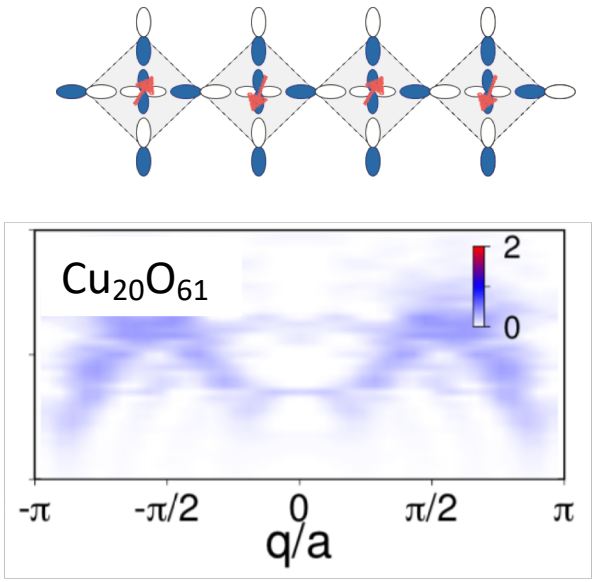

Illustration of a quasi-1D magnetic chain (top) and its magnetic excitation spectrum (bottom). Technical details: A corner-shared CuO_4 chain and its DMRG-based spectrum of the magnetic Cu L-edge RIXS response, using large $Cu_{20}O_{61}$ clusters in the non-spin-flip channel.

A. Nocera, U. Kumar, N. Kaushal, G. Alvarez, E. Dagotto, and S. Johnston, *Sci. Rep*. **8**, 11080 (2018).

This research used computational resources located at UTK/ORNL Joint Institute for Computational Sciences and at NERSC.

Scientific Achievement

Developed new computational approach for improving the resolution of magnetic excitation spectra, using the density matrix renormalization group (DMRG) method for strongly correlated materials.

Significance and Impact

Algorithmic advancements reduce the computational burden, enabling highly accurate calculations for larger and more complex systems that can take advantage of high-performance computing.

Research Details

- Created a DMRG algorithm to calculate resonant inelastic x-ray scattering (RIXS) spectra *exactly* in quasi-1D systems, allowing modeling of the largest systems to date.
- Computed magnetic spectral responses with unprecedented momentum resolution.
- First demonstration that the magnetic RIXS response is well described by a low energy, effective model.