QUANTUM MAGNETS AND MODELS

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EXECUTIVE SUMMARY

Effective models are critical to understanding and simulating the behavior of systems. Examples of effective models include very simple ones, such as ignoring the internal degrees of freedom within a nucleus when considering materials, to very complex ones, like device-level semiconductor modeling. Much of our thinking about materials uses some simplified effective model to make the computations easier, and many of the big successes in materials physics have been the development of high-quality effective models such as the Sommerfeld model, the Bardeen–Cooper–Schrieffer theory for superconductivity, and so on. Meanwhile, due to the continual improvement of high-performance computing resources such as Blue Waters, it is possible to perform amazingly detailed simulations of electronic behavior within materials from first principles knowing only the identity of the atoms involved. We have used these simulations to rigorously connect the detailed simulations to coarse-grained effective models for magnetism.

RESEARCH CHALLENGE

Thanks to the advance of highly parallel and available high-performance computing such as Blue Waters, it is possible to accurately compute the properties of interacting electronic systems using a quantum Monte Carlo method. This technique has been demonstrated on quantum systems of up to 1,000 electrons. While 1,000 interacting quantum particles are challenging to describe, real materials are made up of 10^{23} interacting quantum particles, and so it is imperative to consider multiscale quantum methods. However, the systematic derivation of quantum models from quantum simulations is still under development.

METHODS & CODES

We have developed a new technique that rigorously maps interacting electronic systems from high-accuracy and high-detail quantum simulations to coarse-grained models. This requires quantum Monte Carlo simulations that can compute the one- and two-particle reduced-density matrices. To perform the quantum Monte Carlo calculations, we used the QWalk package developed at the University of Illinois at Urbana-Champaign. QWalk is particularly optimized to use very little memory and to scale almost perfectly to many thousands of cores, and it can compute the necessary observables.

RESULTS & IMPACT

The goal of this work was to produce a prediction of the singlet excitation in the material $MgTi_2O_4$. We have produced a true quantitative prediction in this complex correlated material, which will be checked directly by experiment. In the figure, we show the computed spins, which, when they flip to the same direction, will produce the excitation.

WHY BLUE WATERS

Blue Waters project staff helped optimize the code we used in the calculation. The Blue Waters Symposium (BWS) was an excellent research forum to help us use modern coding practices; for example, we started using Travis CI based on conversations at the BWS.

PUBLICATIONS & DATA SETS

Busemeyer, B., G. MacDougall, and L. Wagner, Singlet-triplet excitation in $MgTi_2O_4$ computed by quantum Monte Carlo. In preparation (2018).

Schiller, J., A. Munoz, L. Wagner, and E. Ertekin, Benchmarking superexchange parameters in the monoxides using quantum Monte Carlo. In preparation (2018).

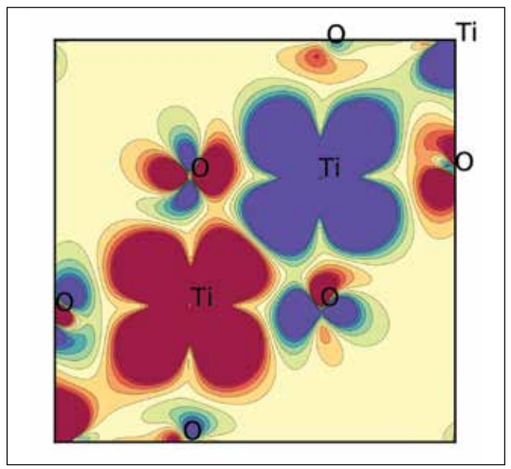

Figure 1: The spin density in $MgTi_2O_4$. Red indicates a net spin-up in a region, while blue indicates a net spin-down. The excitation predicted flips of both spin regions up. The ground state is a quantum superposition of one region up/the other region down with the exchanged configuration.