Usage Report for Fiscal Year 2016

Project Title:

Numerical study of fractional topological phases on two-dimensional lattices

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1. Background and purpose of the project, relationship of the project with other projects

A quantum spin liquid is an exotic state of matter in which strong quantum fluctuation prohibits long-range magnetic order even down to zero temperature[]. So far, various QSL candidates have been found in highly frustrated lattice, such as organic compounds k-(BEDT-TTF)2Cu2(CN)3 and EtMe3Sb[Pd(dmit)2]2 on the triangular lattice and ZnCu3(OH)6Cl2, BaCu3V2O8 etc on the kagome lattice.

Recently, a new QSL candidate YbMgGaO4 was proposed[]. In this material, Yb3+ form a perfect triangular lattice with R3m symmetry. Due to strong spin-orbital coupling effect, the low-energy effective model is a highly anisotropic effective spin-1/2 model:

$$H=\sum_{\langle ij\rangle}[J_{zz}s_i^z s_j^z+J_{\pm}(s_i^+ s_j^- + s_i^- s_j^+)$$
$$+J_{\pm\pm}(g_{ij}s_i^+ s_j^+ + g_{ij}^* s_i^- s_j^-)$$
$$-\frac{iJ_{z\pm}}{2}(g_{ij}^* s_i^+ s_j^z - g_{ij}s_i^- s_j^z)+(i\leftrightarrow j)]$$

where g_{ij} is a bond-denpendent phase.

2. Specific usage status of the system and calculation method

We study the ground state phase diagram of this model by using density matrix renormalization group (DMRG) method. According to the experiment of Li et al[], The parameters in the Hamiltonian take the value $J_{zz}=0.98$, $J_{\pm}=0.90$, $|J_{\pm\pm}|=0.155$, $|J_{\pm z}|=0.04$. Because of the small $J_{\pm z}$, it is convient to ignore this term. We set $J_{zz}=1.00$, $J_{\pm}=0.92$ and study the parameter range $-0.5\le J_{\pm\pm}\le 0.5$. We use the C++ ITensor library running on RIKEN supercomputer GreatWave Hokusai system. We have used all allocated gwacsg and gwacsl resources.

3. Result

We have study many clusters with various sizes. We now show the results for 36 sites cluster as an example.

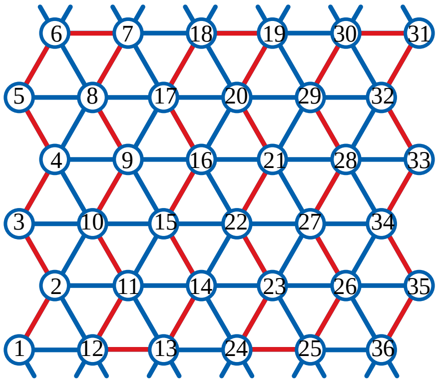

Figure 1. The 36 sites cluster with open boundary condition along x direction and periodic boundary condition along y direction. The red route denote the 1D map in the DMRG calculation.

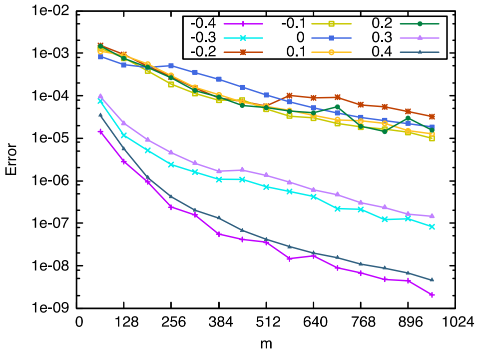

Figure 2. The truncation error as a function of different bond dimension m for various $J_{\pm\pm}$. We see that for small $|J_{\pm\pm}|$ the truncation error is relatively large.

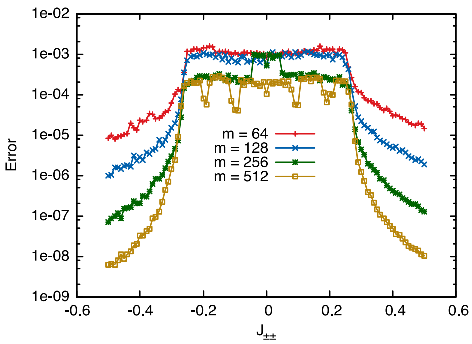

Figure 3. The truncation error as a function of $J_{\pm\pm}$ for various bond dimension m. From this figure, we clearly see that near zero the truncation error is large. It is hard to get accurate results for this parameter range.

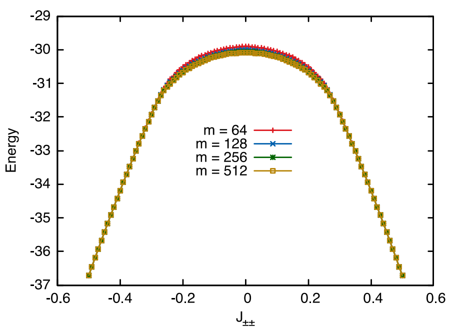

Figure 4. The ground state energy. The first order derivation show no edivence of discontinuity.

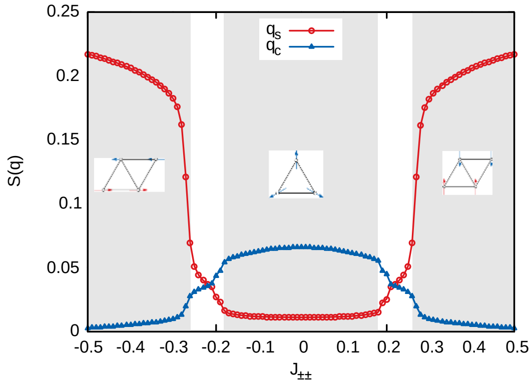

Figure 5. Spin structure factor $S(Q)$. Qs and Qc are order parameter for stripe and 120 degree Neel order phases, respectively. We identify an intermediate region.

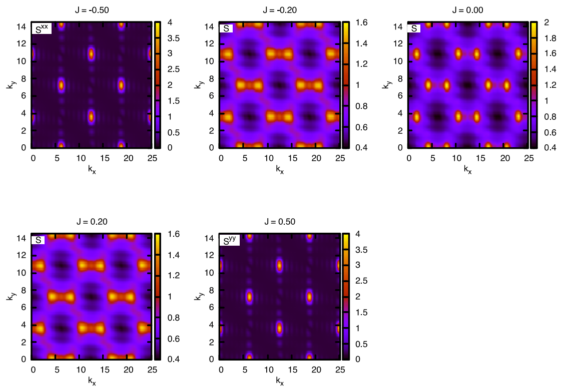

Figure 6. Spin strucutre faction for various $J_{\pm\pm}$. It is evident the identify the stripe order for larger $|J_{\pm\pm}|$ and 120 Neel order with smaller $|J_{\pm\pm}|$.

4. Conclusion

We study a general spin-1/2 model on the triangular YbMgGaO4 lattice. We identify a possible spin liquid phase sandwitched by a stripe phase and a 120 degree ordered phase. Due to limited cluster size, the nature of this spin liquid phase is yet unclear.

5. Schedule and prospect for the future

Latest experiment show that YbMgGaO4 has a spinon Fermi surface[4-5]. We try to investigate the excitation in this model by calculating the dynamical structure factor $S(Q,w)$. It can reveal the nature of quasipartiles and can be directly compared with the experiment data.

References:

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