Usage Report for Fiscal Year 2017

Project Title:

Numerical studies on two-dimensional frustrated quantum spin systems by the DMRG and tensor-network methods

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1. Frustrated quantum spin-1/2 systems provide intriguing possibilities of hosting unconventional nontrivial ground. They may exhibit a quantum spin liquid or valence bond solid behavior showing a quantum entanglement over a long or short distance in a stable phase, respectively, instead of showing a classical long-range order whose ground state can be described by a direct product of local states. By the last fiscal year, we have investigated a spin-1/2 XXZ model on the kagome lattice by using the infinite-size density-matrix renormalization group (iDMRG) method, as well as its three-dimensional generalization, namely, a spin-1/2 XXZ model on the pyrochlore lattice under a [111] magnetic field by using the quantum Monte-Carlo method. The latter work has been published in this fiscal year. (See the reference section.) And we planned to provide theoretical understandings on experimentally realized spin-1/2 kagome antiferromagnets by explaining overall magnetic properties, including the thermodynamic properties and neutron-scattering and electron spin resonance spectra. It is necessary to demonstrate the implementation of the code, in particular, for computing the electron spin resonance spectra. For this purpose, we taken an example of field-induced ferroelectric spin-gapped compound $Rb_2Cu_2Mo_3O_{12}$. As established in Q17308, low-temperature magnetic properties of the material, including the magnetic susceptibility, the inelastic neutron scattering spectra, are explained by a frustrated J_1-J_2 spin-1/2 two-leg ladder model with Dzyaloshinskii-Moriya (DM) interactions, namely $H = H_{\mathrm{SU(2)}} + H_{\mathrm{DM}}$, with the ferromagnetic first-neighbor coupling $J_1 < 0$ and the antiferromagnetic second-neighbor coupling $J_2 > 0$. Here, we focus on the electron spin resonance (ESR) spectra that have recently been measured by experimental collaborators. The ESR spectra from the nonmagnetic ground state of $Rb_2Cu_2Mo_3O_{12}$ below the critical magnetic field ~ 2.0 T are unusually broad, and thus call for a theoretical explanation.

2. The powder-averaged ESR spectra for $Rb_2Cu_2Mo_3O_{12}$, the frustrated J_1 - J_2 spin-1/2 two-leg ladder model with DM interactions, as reported in Q17308, has been investigated by the iDMRG and by the exact diagonalization on a 16-site cluster. We have spent 1.25M hours and 126k hours of CPU time on the MPC and ASCG systems, respectively, by February 15.

We include a magnetic field B through the Zeeman term $H_{\mathrm{Z}} = -g\mu_{\mathrm{B}}\boldsymbol{B}\cdot\sum_{\sigma=\pm;\ell} s_{\sigma,\ell}$ with the g factor $g = 2.16$ which was determined by ESR measurements. The absorption power in ESR measurements for powder samples is approximately given by $I(f,B,T) \propto$

$\frac{B^2 f}{3}\sum_{\alpha'}\sum_{\alpha=x,y,z} S^{\alpha}_{B_{\alpha'},T}(\omega)$, where we introduce the diagonal part of the spin structure factor for $\boldsymbol{Q}=0$ under a magnetic field $B_\alpha = B$ along α axis at a finite temperature T,

$$S^{\alpha}_{B_\alpha,T}(f) = -\frac{1}{\pi}\mathrm{Im}\sum_{\mathrm{k}}\sum_{n} e^{-\frac{E_{B_\alpha,k,n}}{T}} \langle B_\alpha,k,n|S^{\alpha}_{\boldsymbol{Q}=\boldsymbol{0}} \times \left(f+i\eta+E_{B_\alpha,k,n}-H-H_{\mathrm{Z}}\right)^{-1} S^{\alpha}_{\boldsymbol{Q}=\boldsymbol{0}}|B_\alpha,k,n\rangle.$$

Here, $|B_\alpha,k,n\rangle$ and $E_{B_\alpha,k,n}$ are the nth excited state with the wavenumber k along the chain under the magnetic field B_α along α axis and the associated eigenvalue of $H+H_{\mathrm{Z}}$, while the Fourier transform $S^{\alpha}_{\boldsymbol{Q}=\boldsymbol{0}}$ of spin operators in a single two-leg ladder with the number $2L$ of spins is defined by $S^{\alpha}_{\boldsymbol{0}} = \frac{1}{\sqrt{2L}}\sum_{\sigma=\pm}\sum_{\ell=0}^{L-1} s^{\alpha}_{\sigma,\ell}$.

3. We show the theoretical results obtained by the exact diagonalization on a 16-site cluster at 1.6 K in Fig. 1. It shows several modes associated with the transition among $S=1$ triplet excited states that have been split into three by DM interactions. They form two dominant broad spectra below 150 GHz and agree with the experimentally observed broad spectra.

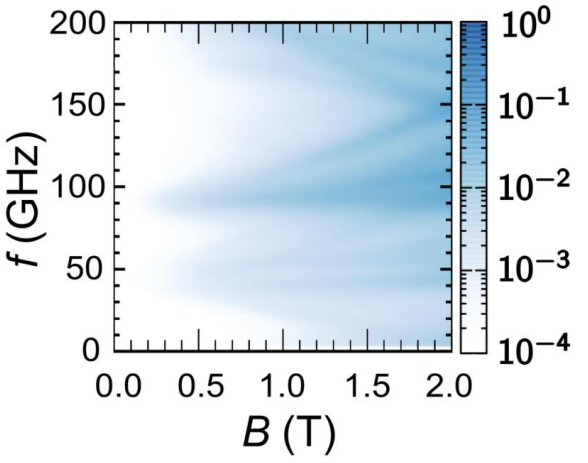

Fig.1: Theoretical optical absorption power at 1.6 K.

4. We conclude that the frustrated J_1-J_2 spin-1/2 two-leg ladder model with DM interactions can nicely explain experimental results of the ESR spectra of $Rb_2Cu_2Mo_3O_{12}$ in the nonmagnetic phase. An origin of experimentally observed broad spectra is attributed to rather large DM interactions.

5. In addition to exact-diagonlization calculations, we have also performed iDMRG calcualtions for computing ESR spectra, since the latter does not suffer from finite-size effects. The results on the lowest-energy part of Fig.1 look similar. However, the computational cost for calculating the higher-energy part was too large for Quick Use. This, as well as an application to two-dimensional frustrated quantum magnets, is left for future study, and will be taken over to a General Project for more generic issues of frustrated quantum magnets in the next fiscal year.

Fiscal Year 2017 List of Publications Resulting from the Use of the supercomputer

[Publications]

Troels Arnfred Bojesen, Shigeki Onoda, "Quantum spin ice under a [111] magnetic field: from pyrochlore to kagomé", Physical Review Letters **119**, 227204 (2017).

[Oral presentation at an international symposium]

Shigeki Onoda, "Quest to U(1) quantum spin liquids, valence bond solids, and novel ordered phases in pyrochlores and spinels: unconventional quasiparticles and interference effects", Junjiro Kanamori Memorial International Symposium (Univ. of Tokyo, Tokyo, Sep. 27-29, 2017). (Invited.)

Troels Arnfred Bojesen, Shigeki Onoda, "U(1) quantum spin liquid and valence bond solid ground states of quantum spin ice under a [111] magnetic field", 28th International Conference on Low Temperature Physics (Gothenburg, Sweden, Aug. 9-16, 2017). (Invited.)

Shigeki Onoda, "Quest to U(1) quantum spin liquids, valence bond solids, novel ordered phases in pyrochlores and spinels: unconventional quasiparticles and interference effects", Topological States and Phase Transitions in Strongly Correlated Systems (Kavli Institute for Theoretical Sciences, Univ. of Chinese Academy of Sciences, Jul. 3-21, 2017). (Invited.)

Shigeki Onoda, "Quantum spin ice under a [111] magnetic field: from pyrochlore to kagomé", Frustrated Magnetism: Conference (Institute of Mathematical Sciences (IMSc), Chennai, India, Apr. 10-12, 2017). (Invited.)

Shigeki Onoda, "Quantum spin ice" Part I, II, and III, Frustrated Magnetism: School (Institute of Mathematical Sciences (IMSc), Chennai, India, Apr. 3-9, 2017). (Invited.)

Hiroshi Ueda, Shigeki Onoda, Yasuhiro Yamaguchi , Tsuyoshi Kimura , Daichi Yoshizawa , Masayuki Hagiwara , Masato Hagihara , Minoru Soda , Takatsugu Masuda , Toshio Sakakibara , Keisuke Tomiyasu , Seiko Kawamura , Kenji Nakajima , Ryoichi Kajimoto , Mitsutaka Nakamura , Yasuhiro Inamura , Masashi Hase , Yukio Yasui, “Emergent spin-1 Haldane gap and ferroelectricity in a frustrated spin-1/2 ladder Rb2Cu2Mo3O12”, APS March meeting, V24.00004, March 8, 2018, Los Angeles, USA.