# §21. Computational Science Study on Quantum Spin Systems by Numerical Diagonalization Method

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Kagome-lattice antiferromagnet is a fundamental system with magnetic frustration. In spite of extensive studies, our understanding of this system is not sufficient due to the limitation of effective methods of analysis. One of the unresolved issues of this system in a magnetic field is the behavior around the one-third magnetization of its saturation.

For such a two-dimensional frustrated system as the kagome-lattice antiferromagnet whose Hamiltonian is given by

$$\mathcal{H} = \sum_{\langle i,j \rangle} J\boldsymbol{S}_i \cdot \boldsymbol{S}_j - H \sum_i S_i^z, \tag{1}$$

it is considered that the numerical-diagonalization method is effective; this method is widely used in various studies. However, several years have been passed since numerical-diagonalization results of the magnetization process of the kagome-lattice system with 36 sites were reported[1)] unless calculations of larger systems have been successfully carried out. In this report, the authors concluded that the magnetization plateau exists at the one-third height of the saturated magnetization $M_s$. However, our careful examination[2)] of the results of the differential susceptibility $\chi$ defined as

$$\chi^{-1} = [E(N, M+1) + E(N, M-1) - 2E(N, M)]M_s, \tag{2}$$

up to 36 sites suggests that the behavior at this height is different from a typical magnetization plateau, where $E(N, M)$ is the lowest-energy of the system with the size $N$ and the magnetization $M$. The new behavior is called the "magnetization ramp."

In order to confirm the behavior of the magnetization ramp, we carry out numerical diagonalization of a system with 39 sites by large-scale parallel calculations using the Plasma Simulator in NIFS[3)]. Our results of the magnetization process and the differential susceptibility are depicted in Fig. 1 and Fig. 2, respectively. Surely, the increase at $M/M_s = 1/3$ is quite small. However, the behavior of $\chi$ is quite anomalous. When one approaches $M/M_s = 1/3$ from the larger-$M/M_s$ side, $\chi$ seems continuous. From the smaller-$M/M_s$ side, on the other hand, $\chi$ shows the divergent behavior. These two phenomena are quite different from the behavior of a typical magnetization plateau in a two-dimensional system.

Our new result of the magnetization process of the kagome-lattice antiferromagnet with 39 sites supports our previous study of the magnetization ramp based on the results up to 36 sites[2)]. The next larger system is a 42-site system. Only the spin gap of this system has recently been reported[4)]. The magnetization process of this system size should be tackled in future studies. Nontrivial ferrimagnetic behavior is also found in the case of the spatially anisotropic interaction[5)]. Numerical-diagonalization calculations of systems as large as possible will provide us with a new and better understanding of condensed-matter physics.

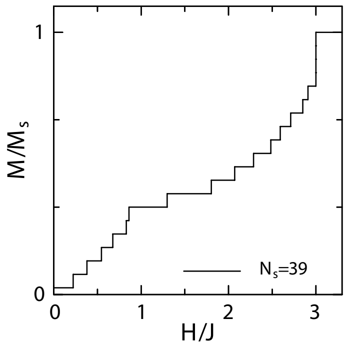


Fig. 1: Magnetization process of the kagome-lattice antiferromagnet with 39 sites.

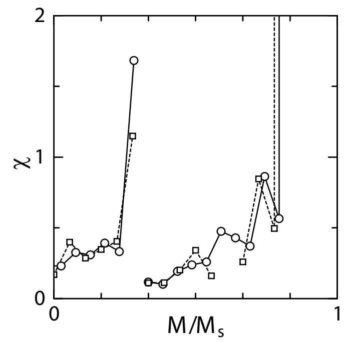


Fig. 2: Differential susceptibility of the kagome-lattice antiferromagnet. Circles and squares denote results of 39 sites and 36 sites.

1) Honecker, A., Schulenberg, J., and Richter, J.: J. Phys.: Condens. Matter **16** (2004) S749.

2) Nakano, H. and Sakai, T.: J. Phys. Soc. Jpn. **79** (2010) 053707.

3) Sakai, T. and Nakano, H.: Phys. Rev. B **83** (2011) 100405(R).

4) Nakano, H. and Sakai, T.: J. Phys. Soc. Jpn. **80** (2011) 053704.

5) Nakano, H., Shimokawa, T., and Sakai, T.: J. Phys. Soc. Jpn. **80** (2011) 033709.