Report on long-term oversea dispatch (1st Aug. 2022 ~ 1st Oct. 2022) Yoshito Watanabe Arima-Tokunaga Laboratory, Department of Advanced Materials Science

Overview

I spent about two months at the University of Cologne, Germany, with Prof. Simon Trebst and group leader Ciarán Hickey. We used two complementary numerical methods, exact diagonalization (ED) and pseudo fermion functional renormalization group (pf-FRG), to study the magnetic phase diagram of the J_1 - J_2 - J_3 spin model (J_n : magnetic interaction in the *n*-th nearest neighbor) on a honeycomb lattice. This report presents what I have done during this long-term oversea dispatch.

Summary of Research

The two-dimensional honeycomb lattice is a system in which strong quantum effects exist due to the small coordination number of 3 for each site. Recently, it has been theoretically proposed that the Kitaev model, which is an exactly solvable quantum spin model on a honeycomb lattice, can realize a quantum spin liquid state, and intense experimental searches for the candidate material have been performed. It has been reported, however, that some of the Kitaev candidate materials are rather well described by another model, the J_1 - J_2 - J_3 spin model. The classical J_1 - J_2 - J_3 spin model has been studied for a long time. It is known that there is an exact correspondence



Fig. 1 A photo taken with the member of the Institute for Theoretical Physic. Behind is a statue of Albertus Magnus, who is a founder of the University of Cologne.

between the ferromagnetic $(J_1 < 0)$ and antiferromagnetic $(J_1 > 0)$ nearest neighbor interactions under a zero magnetic field. Although this correspondence does not hold for quantum spin systems, existing studies have focused mainly only on the antiferromagnetic $(J_1 > 0)$ case. In this study, we investigate the magnetic phase diagram of the quantum spin J_1 - J_2 - J_3 model using ED and pf-FRG. ED is a powerful numerical tool to obtain wavefunctions of the ground and excited states, which define the properties of the quantum spin system. On the other hand, the number of sites that can be handled by a computer is relatively small, which requires careful handling of finite-size effects and is incompatible with incommensurate magnetic ordering. Although pf-FRG has limited access to information compared to ED, it can handle a larger system size, allowing high momentum spin systems by using ED and pf-FRG in a complementary manner.

One of the main results of this work is that we have obtained an intriguing magnetic phase diagram for systems with ferromagnetic nearest-neighbor interactions ($J_1 < 0$), which have not been well investigated previously. In addition to the magnetic phases reported for classical spin

systems, we have discovered a quantum phase that shows no clear signs of long-range order; the ED results suggest that the energy gap in this phase is very small, suggesting a gapless quantum spin liquid state. We have also found that when easy-plane type anisotropy is introduced into the interaction, this spin liquid phase evolves into a spiral-ordered phase which is also observed in the classical spin counterpart. These results will be summarized in a paper.

Living in Cologne

Cologne, located on the Rhine River in western Germany, is known for its changeable weather, but for the first month after my arrival, the weather was dry and almost rain-free. Especially the first two weeks were very tough, with highs in the upper 30s Celsius and no air-conditioning inside the rooms. There seemed to be some concern about water shortages in Germany. On the other hand, in September, the weather returned to normal, and the weather was pleasant, albeit rainy.

I spent weekday afternoons and holidays running as Cologne has many lush greenery parks. Later, it turned out that Prof. Simon also happened to run in the same places often, and he further introduced me to some recommended running spots and local running events. I participated in one of the running events. Unfortunately, the result was unsatisfactory, so I would like to continue improving my running skills.

On weekdays, I usually had lunch at the mensa (cafeteria), where people from different research groups in the same building gathered. During my stay (in August and September), the number of dishes on the menu was smaller than usual, as there were no classes. Still, it is impressive to me



Fig. 2 A scene from a running event I participated in at the site. The weather that day was typical of Cologne, with rain and sunshine switching rapidly in a short period.

that there were more vegetarian dishes on the menu than non-vegetarian ones. According to what I have heard, in recent years, more and more people in Germany are reducing meat consumption and becoming vegetarian due to animal welfare, environmental protection, and health considerations. In fact, many of the group members were also cutting back on meat consumption. We may see such a trend in Japan in the future.

Acknowledgement

For this stay, I would like to thank "Quantum Liquid Crystals" for the financial support. I would also like to thank my advisor, Professor Takahisa Arima, my secondary advisor, Professor Takasada Shibauchi, and the MERIT program for allowing me to go abroad for a long time. As an experimentalist, I was worried about whether I could learn and achieve something in a very short period of two months. But after all, I could spend a fulfilling time during my stay thanks to the conscientious and kind assistance from Prof. Simon Trebst and Ciarán Hickey group leader, which allowed me to spend a fulfilling time during my visit. So here, I would like to thank them and their group members again.