Report of MERIT Long-term Overseas Dispatch

Department of Applied Physics (D3)

Kensaku Takai

title : investigation of metal-insulator transition by variational Monte Carlo method

1. Outline of my long-term overseas dispatch

I stayed at Julius-Maximilians-University Würzburg from February 1st to March 28th and researched with Prof. Fakher Assaad and the members of his group.

2. Background of my research

It is known that metal-insulator transition (Mott transition) is a common phenomenon in high-temperature superconductors of cuprates, and it occurs at the temperatures and pressures close to superconductivity in organic conductors. Though metal-insulator transition is closely related to high-temperature superconductivity, it has been difficult to treat it accurately with taking into account of long-ranged fluctuations of charge density (spatial correlations). Prof. Fakher Assaad is one of the top researchers of critical and topological phenomena with electron correlations. He and his group have improved quantum Monte Carlo (QMC) method and cluster dynamical mean-field theory (CDMFT), and applied them to critical phenomena in the quasi-one-dimensional Hubbard models (dimensional crossover) recently. However, CDMFT partly disregard spatial correlations, so the transitions become Slater transitions with antiferromagnetic orders.

3. Research collaboration and our results

In Imada group, we have developed the many-variable variational Monte Carlo (mVMC) method, the high-accuracy and high-efficiency computational method without the negative sign problem for ground state calculations. Furthermore, I and my coworkers have developed the finite-temperature variational Monte Carlo (FT-VMC) method by combining with the time-dependent variational principle (TDVP) for finite-temperature calculations. During my stay in Würzburg, I applied mVMC to metal-insulator transitions in quasi-one-dimensional Hubbard models, and I calculated various physical quantities, for example, double occupancy, the momentum distribution function and the spin correlation function. In addition, I performed size extrapolations of spin correlation function to judge the type of transitions. As the results, we obtained the phase diagram of mVMC that is different from that of CDMFT. I plan to perform calculations for critical exponents at large system sizes and finite temperatures by

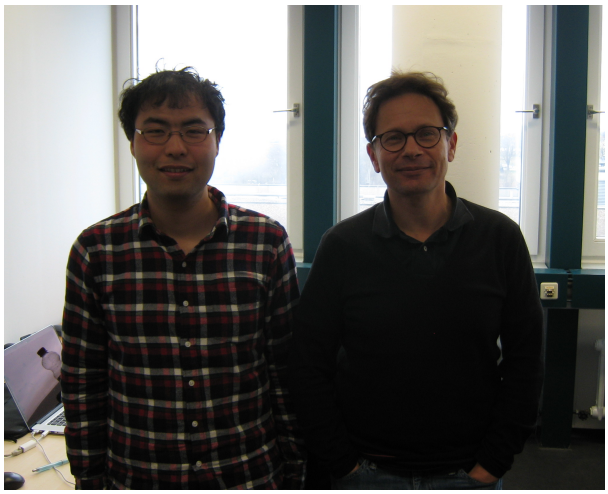
FT-VMC. We continue to take contact with Prof. Fakher Assaad and Dr. Marcin Raczkowski (my coworker) three or four times a month for discussions by Skype.

4. About my research life

Würzburg, located between Frankfurt and Nürnberg, is a small city with a population of 130,000 people. There are wide grape fields in Würzburg and it is the center of Franken wine production. In addition, the Würzburg residence is registered as the world heritage and this city is the starting point of the romantic road, so it is one of the famous sightseeing spots for Japanese tourists. Public transportations of Würzburg are only buses and trams, and I commuted to the university by bus every day. I had worked from 9 to 19 o'clock owing to short sunlight hours in winter. The members of Assaad group speak English fluently, but bus drivers and shop clerks speak only German. Hence, I had to make efforts to communicate with them. During my stay, I went to Regensburg for joining in Deutsche Physikalische Gesellschaft (DPG) with members of Assaad group. In addition, I joined in the internal meeting of strongly correlated electron systems and I had an opportunity to talk with other German students in the poster session.

5. Acknowledgments

I thank Prof. Fakher Assaad, Ms. Özge Özoglan (the secretary of theoretical physics I), Dr. Marcin Raczkowski (my coworker), and Assaad group members for supporting my research and daily life. I also thank Prof. Masatoshi Imada and Dr. Yohei Yamaji for advising me through may stay in Würzburg. Finally, I appreciate MERIT program and Prof. Koichi Yamashita (my vice supervisor) to admit me to go to Germany.



with Prof. Fakher Assaad