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Bilateral International Exchange Program (BIEP, invite) report

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(Year/Month/Day)_____

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Research Project

Title	Transport in One-Dimensional Quantum Systems at Finite Temperatures
Duration	June 20, 2009 – July 20, 2009

On the first day of my stay in Kyoto University I gave a seminar about my previous work with prof. Prelovsek regarding the combination of Finite temperature Lanczos method and Density matrix renormalization group (FT-DMRG). That has clarified the current status of the FT-DMRG and was a good starting point for further development.

Due to the capability of FT-DMRG for treating one dimensional (1D) systems we decided to look for real materials which show the 1D behavior, among which, many materials reflect spin frustrations with pronounced quantum mechanical fluctuations and are therefore in the center of interest of many condensed matter researchers. Synthesis of materials like $GeCuO_3$ and $TlCuCl_3$ has attracted much attention, since they might be well described with 1D Hamiltonians.

The subsequent work was devoted to literature research to evaluate the current status of the knowledge about these materials and to consider some open questions. We found that dynamics of $GeCuO_3$ was not treated theoretically at finite temperatures and that experimental results are still not well understood and that there is still no agreement about the corresponding microscopic model.

Then we focused on code development. First we had to code the corresponding Hamiltonian, which is a J_1-J_2 Heisenberg Hamiltonian including also dimerization. Treatment of transport properties like spin current or heat current and treatment of dynamics like dynamical spin structure factor needed also an inclusion and coding of spin current operator, which is an extension of somehow simpler operator for treating chirality (currently a hot topic). Another operator, which we included, is a spin structure factor operator.

During the code development a lot of testing was preformed, which was mainly done with comparison of results with parallel work of graduate student Sugimoto, with whom also a lot of technical details were discussed, e.g. coding of spin current operator for system and environment block in the process of DMRG, and was beneficial for both sides. Codes were firmly tested, together with convergence of results due to some parameters, which showed better solutions and also raised a confidence in the validity of results.

In the following we focused on calculation of physical properties, e.g. spin transport and dynamical structure factor at finite temperatures, aiming to explain the experimental data and to make some theoretical predictions. Current results of the dynamical spin structure factor for $GeCuO_3$ are promising and show good agreement with the experiment, although some features are missing, which might be interesting for discussion of relevant terms of the microscopic model as well as relevant physical phenomena.

However, obtaining results relevant for physical society demands serious and larger scale calculations with carefully chosen optimal parameters and that takes more time. Our latest work was devoted to search of such parameters, preparation for final calculations and also some steps were made towards the presentation of results.

Our future cooperation with prof. Tohyama will be devoted to finalizing this work and to present results to wider audience by publishing them.