Project Title:

Highly correlated study of the FeSe single layer: probing structural and superconducting properties with quantum Monte Carlo

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In this project, we use Quantum Monte Carlo (QMC) for studying the properties of Iron Based Superconductors (IBS) in order to establish whether they can be understood in terms of a variational wave function that describes strong electron correlation and that can give rise to superconductivity even outside the conventional electron phonon mechanism, based on the BCS theory.
This project is very challenging and is a continuation of a previous projects in RIKEN-HOKUSAI.
In this first period, we have already obtained encouraging results in the description of magnetic properties, a very difficult subject, because near the superconductivity transition several structures become competitive in energy and may explain the experimental observation of a paramagnetic Iron-Selenide material with maximum T_c at a pressure of about 10 GPa.
These results have been published in the Physical Review B **94** 035108, where we show that the computational method we are using (the TurboRVB package) provides the lowest variational energies and allows the structural optimization, that is so important in these systems. For instance, it was observed in several experiments a clear correlation between T_c and the height position of the Se atom.

In parallel, we developed new strategies to reduce the finite-size scaling. In particular, we proposed a simplified version of the k-point sampling, which is based on a special twist (special k-point), giving the exact thermodynamic limit in non-correlated calculations. This approach can be very important to study systems with large unit cells and to optimize the determinantal part of the wave function. The special k-point was already known in the density functional theory community, but it has never been exploited in correlated QMC calculations. To test this scheme in QMC, it was fundamental to use the computational resources available in HOKUSAI, as we had to show the convergence properties of different methods by simulating large systems, requiring heavy computational use. The results of this work have been published in the Physical Review B **94,** 245108.

Both steps undertaken this year, namely the study of different magnetic patterns and their relation with the geometry in bulk FeSe, and the methodological development to reduce finite-size effects, are both necessary to reach the final goal of simulating the FeSe monolayer, the ultimate target of this year proposal. Unfortunately, we have not been able to carry out calculations of FeSe monolayer, as we have been busy with those previous propaedeutic steps.

In conclusion, though the computational QMC method requires large computer resources and high performance supercomputers, such as the one provided by the HOKUSAI infrastructure, we believe that is worth continuing with this project with the final purpose to understand also the superconducting properties of these materials, and, possibly, all strongly correlated high critical temperature superconductors, such as the Cuprates and the recently discovered Hydrogen-Sulfur compounds. The human and computational time spent this year in HOKUSAI makes up another advancement toward the final goal of understanding unconventional superconductivity in IBS and related materials from first principles.

Fiscal Year 2016 List of Publications Resulting from the Use of the supercomputer

[Publication]

Brian Busemeyer, Mario Dagrada, Sandro Sorella, Michele Casula, and Lucas K. Wagner, **"Competing collinear magnetic structures in superconducting FeSe by first-principles quantum Monte Carlo calculations"**, Physical Review B **94,** 035108 (2016);

M. Dagrada, S. Karakuzu, V. L. Vildosola, M. Casula, S. Sorella, **"Exact special twist method for quantum Monte Carlo simulations"**, Physical Review B **94**, 245108 (2016).

[Oral presentation at an international symposium]

What about U? ICTP, 17-21 October 2016, invited talk;
Workshop on "Matériaux, États Électroniques, Interactions et Couplages non-Conventionnels", invited talk
"Quantum Monte Carlo methods for strongly correlated systems from first principles", June 2016, Paris (France);