Development of open-source software for Many-variable variational Monte Carlo (mVMC) method

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The variational Monte Carlo (VMC) method is a commonly used method for treating the low-energy effective models of quantum many-body systems such as the Hubbard model and the Heisenberg model [1]. In the VMC method, the many-body correlation factors such as the Gutzwiller and the Jastrow factors are introduced to the one-body wave functions. By optimizing the variational parameters in the many-body wave functions to lower the energy, we can obtain the wave functions for the ground states of the quantum many-body systems.

Because the VMC does not suffer from the negative sign problems, the VMC method is widely used for analyzing the low-energy effective models for quantum many-body systems including the strongly correlated electrons systems. However, it has been pointed out that accuracy of the conventional VMC method is not high due to the strong limitation of the implemented wave functions in the conventional VMC method. To overcome the limitation of the conventional VMC, we have introduced many variational parameters in the one-body part of the wave functions (typically more than ten thousand variational parameters) and have succeeded in relaxing the limitations of the wave functions. We also employ the quantum number projection to recover the symmetries inherent to the systems [2]. By combining the many-variable variational wave functions and the quantum number projections,

we have shown that the highly accurate calculations is possible for the wide range of the quantum many-body systems [2, 3]. We call this method *many-variable variational Monte Carlo* (mVMC) method to distinguish the conventional VMC method, whose number of variational parameters is limited to more or less one hundred. Although the optimization of the many variational parameters is difficult in general, it is shown that the optimization of more than ten thousand variational parameters is possible by using the stochastic reconfiguration (SR) method proposed by S. Sorella [4], which is based on the imaginary-time evolution of the wave functions.

The project for advancement of software usability in materials science in the 2016 fiscal year has supported the release of the mVMC as the open-source software [5]. The project has especially supported the improvement of the user interfaces of mVMC and extensions of the wave functions. The latest version of the mVMC is preinstalled on the system B (sekirei) of the supercomputers at ISSP.

By using the software, users can easily start the mVMC calculation by preparing one input file, whose length is typically less than ten lines, for the standard models in the strongly correlated electron systems. As an example, we show the input file for the 4×4 Hubbard model as below:

```
L       = 4
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```
W       = 4
Lsub    = 2
Wsub    = 2
model   = "FermionHubbard"
lattice = "tetragonal"
U       = 4.0
t       = 1.0
nelec   = 16
```

Here L and W are a linear extents of square lattice, in x and y directions, respectively. The nearest neighbor transfer (on-site Coulomb repulsion) is represented by t (U). Details of the other keywords in the input files can be found in the manuals of mVMC [5]. In Fig. 1, we show the optimization process of the mVMC. As shown in this figure, by preparing the above simple input file, users can easily obtain the wave functions for the ground state whose accuracy is $E_{\mathrm{mVMC}} - E_{\mathrm{exact}} \sim 10^{-3} \times t$. By changing the keywords in the input file slightly, users can easily perform the mVMC calculations for the other standard models such as the Heisenberg model and the Kondo-lattice model. It is also easy to treat more general models in the quantum many-body systems by properly preparing the input files. We hope that the mVMC becomes useful software and will be widely used by the broad spectrum of the researchers in the condensed matter physics as well as the other fields such as the quantum chemistry.

Figure 1: Optimization process of mVMC for 4×4 Hubbard model. The internal energy per site calculated by mVMC (exact diagonalization) is represented by E_{mMVC} (E_{exact}). Exact diagonalization is done by using $\mathcal{H}\Phi$ [6]. We take two different initial states: One is the random initial states (red crosses) whose initial variational parameters are generated by the random numbers and the variational parameters of the another one is generated by results of the unrestricted Hartree-Fock (UHF) calculations (blue circles). Although the two different initial states give nearly the same converged results, the convergence is faster by taking UHF initial states.

References

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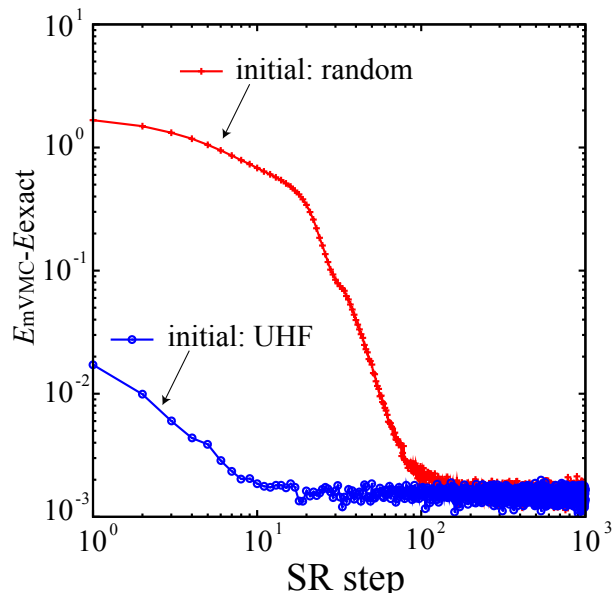
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