

Massively parallel variational Monte Carlo method for excitation spectra augmented by artificial neural networks

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We have extended the dynamical variational Monte Carlo (dVMC) method [1, 2] for dynamical structure factors to simulating photoemission/inverse photoemission and resonant inelastic x-ray scattering spectra. In Fig. 1, the charge and spin dynamical structure factors (left panel) and momentum resolved inverse photoemission spectrum (right panel) for a one-dimensional half-filled Hubbard model are shown as examples of the extended dVMC results. By combining the results of the dynamical structure factors and the inverse photoemission, we can obtain the resonant inelastic x-ray scattering spectrum as well.

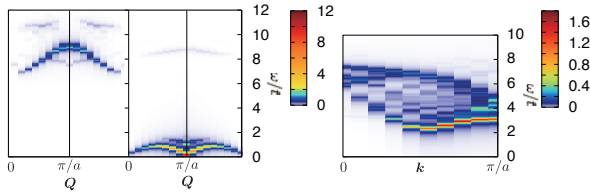


Figure 1: Examples of dVMC results for the one-dimensional Hubbard model at half-filling with 18 sites.

In the present project, we have introduced the quantum number projections [3] omitted in the previous version of the dVMC [2], to improve the accuracy and efficiency of the shared memory parallelization. To further improve the accuracy of the numerical spectroscopy realized by the dVMC method, we also incorporate the restricted Boltzmann machine, which

was implemented in the original mVMC [4], and the feed-forward deep neural network, as a part of the generalized Jastrow-Gutzwiller correlation factor.

By further analyzing the resonant inelastic x-ray scattering simulation, we can identify the mutual correlations between single-particle spectral weight and charge and spin excitations. In the one-dimensional Hubbard model, for example, the correlations indeed enable us to identify the spinon and holon branches.

We will apply the method developed in the present project to the low-energy *ab initio* hamiltonians for the cuprate superconductors. To improve the parallelization efficiency of the present dVMC method, the population Monte Carlo that may shorten the warming up process will be useful.

References

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