Usage Report for Fiscal Year 2024

Project Title:

Implementing the Gutzwiller wave function for SU(3) fermions

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1. Background and purpose of the project, relationship of the project with other projects

The Gutzwiller-projected state is defined by projecting a non-interacting trial state to impose the single-occupancy constraints on each lattice site. Despite its simplicity, the Gutzwiller-projected state effectively captures important interaction-induced phenomena.

We generalized the linear-combination-of-unitary (LCU) method, proposed by K. Seki et.al., from SU(2) fermionic systems to SU(3) fermions. The corresponding Gutzwiller wave function can be employed to investigate the novel phase transition in attractive SU(3) Hubbard model.

Two complementary approaches are reformulated to perform the sum in the LCU formula. Specifically, the second approach utilizes the importance sampling technique to solve the Gutzwiller variational problem where the expectation values of observables are the central objectives. A part of the numerical simulations is performed using the HOKUSAI supercomputer.

2. Specific usage status of the system and calculation method

For the importance sampling approach, we design the Monte Carlo simulation to generate the sequence of auxiliary fields that represent samples drawn from a probability. The Monte Carlo simulations is performed without the phase problem, and the results are averaged over 16 CPU cores with 2000 warmup sweeps and 2000 measurement sweeps.

3. Result

We calculate the energies and the triple occupancy per site for the 4-site one-dimensional chain under open boundary conditions and 2 by 2 square lattice. The results obtained by fully summing all auxiliary fields and using the importance sampling approach agree with the exact results within the statistical errors.

4. Conclusion

In summary, we generalized the quantum-classical hybrid scheme that prepares the Gutzwiller wave function to the attractive SU(3) fermion systems. We reformulated two complementary approaches that perform the sum over the auxiliary fields: The first approach is probabilistic, leveraging the ancillary qubits in the linear-combination-of-unitary circuit to prepare the Gutzwiller wave function on the quantum computer; the second approach uses the importance sampling technique to evaluate the expectation values for the Gutzwiller wave function stochastically. We tested these two approaches for small-size lattices, calculating the expectation values of energies and triple occupancy as a function of the Gutzwiller variational parameter.

5. Schedule and prospect for the future

Extensions of the present experiments on larger lattices, to study the pairing and trion formations in attractive SU(3) fermion systems, will be worth studying in the future.

6. If no job was executed, specify the reason.

Fiscal Year 2024 List of Publications Resulting from the Use of the supercomputer

[Poster presentation]

Title: Preparing Gutzwiller wave function for attractive SU(3) fermions on a quantum computer
Author: Han Xu, Kazuhiro Seki and Seiji Yunoki

Name of the meeting: SU(N) physics in quantum many-body systems: theory, experiment, and numerics (SUN2024)

Presentation date: Jul. 11, 2024

Place: Online poster sessions