Many-body quantum simulations based on multi-scale space-time ansatz

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We have worked on the following topics in collaboration with co-workers.

(1) Parallelization quantics tensor train

We have implemented Julia libraries (TensorCrossInterpolation.jl, QuanticsGrids.jl) [1] for tensor cross interpolation and quantic tensor train [2,3]. A critical step toward practical calculations is parallelization of the algorithm. We have implemented a prototype parallelized code based on quantics tensor train in Julia. The code is still experimental and to be benchmarked on a HPC system.

(2) Hidden covalent insulator and spin excitations in SrRu2O6

We applied the density functional+dynamical mean-field theory to study the spin excitation spectra of SrRu2O6. We used DCore [4] and ALPS/CT-HYB [5]. After computing a self-consistent solution, we solved the Bethe-Salpeter equation to compute the dynamical susceptibility.

We found a good quantitative agreement with experimental spin excitation spectra. Depending on the size of the Hund's coupling J_H, the system chooses either the Mott insulator or covalent insulator state when magnetic ordering is not allowed. We found that the nature of the paramagnetic state has a negligible influence on the charge and spin excitation spectra.

(3) Comparative study of variational quantum circuits for quantum impurity models

We have developed compact ansatz for solving quantum impurity models using variational quantum circuits [7]. Our approaches are based on two ideas. First, we employed a compact physics-inspired ansatz, *k*-unitary cluster Jastrow ansatz, developed in the field of quantum chemistry. Second, we eliminated largely redundant variational parameters of physics-inspired ansatz associated with bath sites based on physical intuition. We benchmarked the new ansatzes and found that the compact anstazes outperform the original ansatz in terms of the number of variational parameters.

(4) Classical Monte Carlo simulation of J_1-J_2 *XY* Kagome antiferromagnet

We investigated the J_2-T phase diagram of the J_1-J_2 *XY* Kagome antiferromagnet using extensive classical Monte Carlo simulations based on non-local loop updates and replica-exchange Monte Carlo method [8]. Our code is implemented in Julia and use MPI parallelization. The obtained phase diagram

features Berezinskii-Kosterlitz-Thouless transitions of $q = 0$, $\sqrt{3} \times \sqrt{3}$ magnetic orders, and octupole orders, in addition to finite-temperature phase transitions of both ferrochiral and antiferrochiral long-range orders. We found a nontrivial first-order transition for antiferromagnetic $J_2/J_1 < 0$.

References

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