Development of COMPutation ARchive of Exact Diagonalization (COMPARED)

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Development of accurate numerical solvers for quantum many-body systems is one of the central issues in the field of computational materials sciences. To achieve this goal, the exact diagonalization method has been widely used for benchmarks on the systems smaller than 50 sites because this method enables us to obtain numerically exact results in the systems with arbitrary interactions. Although most numerical data obtained by the exact diagonalization method are available on articles, these representations such as definition of the Hamiltonians and the display digits of the results are dependent on the articles. Therefore, it is desirable for construction of database to easily check and obtain the exact diagonalization results without definition of notations.

In this project, we have constructed an open database for exact diagonalization results, which is called "COMPutation ARchive of Exact Diagonalization (COMPARED)" [1]. This database has been available on the ISSP data repository under the CC BY 4.0 license [2]. As a generator of the exact results, we use open-source software HPhi [3], which supports MPI/OpenMP hybrid parallelization to achieve highly efficient simulations on supercomputers. Although this parallelization is efficiently done for large system sizes such as 36 sites of quantum spin systems, it is not for single parameter set for small system sizes. To generate data for small system sizes, we develop a python tool which performs HPhi's simulations parallelly. This tool parallelizes input parameter sets and performs the simulations independently for each parameter set. Now we have released more than 20 million data focused on the energies of the ground state and the first excited state on quantum spin systems with small system sizes [2]. We will upload the results for large systems and electron systems.

This project has been done in collaboration with Kazuyoshi Yoshimi and Yuichi Motoyama.

References

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[3] M. Kawamura, K. Yoshimi, T. Misawa, Y. Yamaji, S. Todo, and N. Kawashima: Comp. Phys. Commun. **217** (2017) 180.