Development of numerical library Kω ver.1 and quantum lattice solver $\mathcal{H}\Phi$ ver.2

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The two novel open-source softwares of (i) numerical library Kω ver.1 [1] and (ii) quantum lattice solver $\mathcal{H}\Phi$ ver.2 [2] were developed in Project for advancement of software usability in materials science [3] at the fiscal year of 2016. The project name is 'shifted Krylov-subspace algorithm and novel solvers for computational condensed matter physics'. The project is a interdisciplinary one between computational material science and applied mathematics. The softwares are preinstalled on the supercomputer (Sekirei) at ISSP [3]. The two softwares are closely related, because Kω is a set of numerical linear-algebraic routines and $\mathcal{H}\Phi$ ver.2 supports the use of Kω in the optical spectrum calculations.

Kω is a general numerical library for the Green's function of

$$G^{ab}(\omega) = \langle a| \frac{1}{(E_0 + \omega + i\delta)I - H} |b\rangle, \qquad (1)$$

where H is a large-scale complex-Hermitian or real-symmetric matrix and $|a\rangle, |b\rangle$ are the input vectors. Traditionally, the problem was solved by the Lanczos-based algorithm. In the present solver, instead, the numerical solution of Eq. (1) is obtained from the linear equation of

$$[(E_0 + \omega + i\delta)I - H]\,|x\rangle = |b\rangle \qquad (2)$$

and the solution of $|x\rangle$ is obtained by the novel iterative algorithm, called shifted Krylov-subspace algorithm [4, 5]. The algorithm was used for the excited spectrum of many-body states in a previous paper [5], which motivated us to the present project. The algorithm enables us to control the accuracy of the spectrum $G^{ab}(\omega)$ at a specific frequently ω [5], when one monitors the residual vector of Eq. (2). The method is general and was applied also to many other computational science fields, such as QCD[4], electronic structure calculations, transport calculation with non-equilibrium Green's function theory. Kω is a general numerical library and can be called, in principle, from any material simulator, as well as $\mathcal{H}\Phi$ ver.2. Moreover, a mini-application is included in the package of Kω, so that researchers can evaluate the numerical library before the use in their real researches.

$\mathcal{H}\Phi$ ver.2 is the latest version of $\mathcal{H}\Phi$ [6]. The quantum lattice solver $\mathcal{H}\Phi$ is a program

package based on exact diagonalization applicable to a broad range of quantum lattice models, including the Heisenberg model, the Kitaev model, the Hubbard model and the Kondo-lattice model. In $\mathcal{H}\Phi$ ver.1, the Lanczos method for calculating the ground state and a few excited states, thermal pure quantum (TPQ) states [7] for finite-temperature calculations, and full diagonalization method for checking results of Lanczos and TPQ methods are implemented with an easy-to-use and flexible user interface.

The project in the 2016 fiscal year [3] has supported implementation of the Lanczos and shifted Krylov-subspace algorithm for calculating excitation spectra in the latest version $\mathcal{H}\Phi$ ver.2. The $\mathcal{H}\Phi$ ver.2 call subroutines for the shifted Krylov-subspace algorithm from the library Kω.

As an example tractable by $\mathcal{H}\Phi$ ver.2, we show excitation spectra of an *ab initio* spin hamiltonian of an iridium oxides Na_2IrO_3 [8], which is a so-called Kitaev material and a typical example of frustrated magnets due to magnetic anisotropy. In Fig.1, dynamical spin structure factors calculated for a 24-site cluster of the *ab initio* spin hamiltonian of an iridium oxides Na_2IrO_3 are shown. The continuum in the spectra is the hallmark of the proximity to the Kitaev's quantum spin liquid. The controlled accuracy of the shifted Krylov-subspace algorithm safely resolves the detailed continuum spread over the wide range of frequency, where the typical exchange energy scale of Na_2IrO_3 is 30 meV.

For a future outlook, the successor project in the fiscal year of 2017 [3] will support implementation of real-time dynamics, finite-temperature excitation spectra, and interfaces for data science approaches.

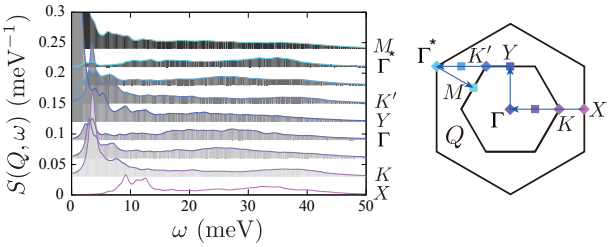

Figure 1: Calculated dynamical structure factors $S(Q,\omega)$ of Na_2IrO_3 [8]. The spectra are vertically shifted depending on Q. The Brillouin zone of Na_2IrO_3 is shown in the right panel.

References

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