Machine learning and *ab initio* analyses of cuprate high-temperature superconductors

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Understanding physics of high-T_c cuprate superconductors remains one of the challenges in physics. In this project, we have continued efforts to clarify physics and mechanism of high-temperature superconductivity, particularly for the copper oxides. This is a combined research activity of three different approaches:

(1) Parameter search of strongly correlated electron models by using high-accuracy solvers for quantum many-body lattice Hamiltonians

(2) Parameter-free *ab initio* studies of real materials by using multi-scale *ab initio* scheme for correlated electrons (MACE) [1]

(3) Data science approaches to expose hidden physical quantities and mechanisms by combining extended experimental data such as by angle resolved photoemission spectroscopy (ARPES), quasiparticle interference (QPI) by scanning tunnel microscope (STM) and resonant inelastic X-ray scattering (RIXS) with the help of applied mathematical and information science technology such as machine-learning tools.

In the first approach, we have continued to clarify physics of electron fractionalization and formation of topological states such as quantum spin liquids (QSL). It was achieved by using the variational Monte Carlo tools (mVMC) [2] combined with the restricted Boltzmann machine developed by us [3,4], tensor network [5,6] and the Lanczos diagonalization. In the J_1-J_2 Heisenberg model defined on the 2D square lattice with the nearest neighbor exchange interaction (J_1) and the next nearest neighbor exchange (J_2), we have further firmly established the existence of the QSL in the region $0.49<J_2/J_1<0.54$ [7]. The analyses were elaborated by comparing the accuracy of our solver with other tools in the literature. The accuracy and reliability of our solver were shown to be the best among existing solvers both for the ground states and the excitations. The reliability and robustness of the analyses was confirmed by (i) the size insensitivity of the correlation-ratio crossing points to identify the QSL-antiferromagnetic transition and the QSL to valence-bond-solid transition (ii) the insensitivity about the choice of the initial variational parameters for the wavefunction (iii) better size extrapolation of the level crossing point to infer the ground state phase boundary

from the level crossing points of the excitation spectra, where larger size calculation has been added to enhance the accuracy of the extrapolation.

We have also been investigating the quantum ground state of the S=1/2 Heisenberg antiferromagnet on the pyrochlore lattice [8]. After investigation of various trial wave functions, we find that the singlet ground state has a linear dispersion at vanishing momentum with a finite energy gap to triplet excitations. Furthermore, it has turned out that the ground state is fully degenerate for all the point group symmetry represented by the irreducible symmetry group, which implies an emergence of the unprecedented type of quantum spin liquid.

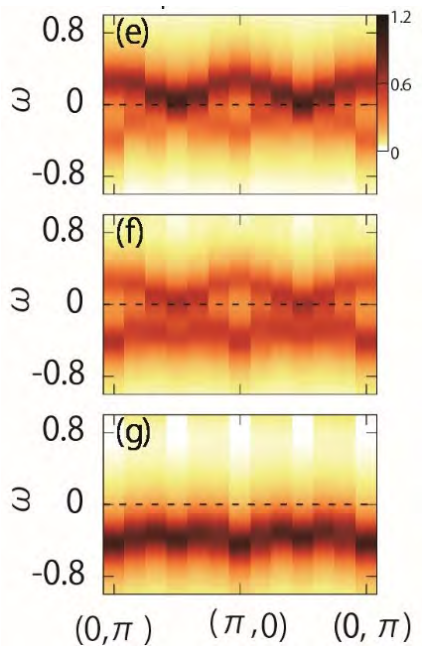

Fig.1: Spectral function along around symmetry line. (f) is closest to the symmetry line showing a large d-wave gap at (π,0) [10].

Accurate algorithms and tools for quantum dynamics were also sought for [9]. A method to calculate spectral functions measurable by the ARPES representing the imaginary part of the electron single-particle Green's function was developed in addition to the two-particle dynamical structure factor for spin and charge [10]. The application to the Hubbard model revealed the d-wave gap structure for the first time in the superconducting state as shown in Fig.1. It has shown an unrealistically large gap of the typical Hubbard model implying an oversimplified nature of the Hubbard model as a model of the cuprate superconductors.

For the *ab initio* approaches (2), we have reproduced the experimental phase diagram of $HgBa_2CuO_{4+y}$ [11] by solving its *ab initio* low-energy effective Hamiltonian without adjustable parameters [12]. Thanks to this success, in the present project in 2020, more thorough and systematic analyses for several different copper oxide compounds have started. Derivation of *ab initio* low-energy effective Hamiltonians for the series of multi-layer compounds including Bi and solving with refined mVMC tool is under way.

The third data science approach (3) has been elaborated for the machine learning analysis of the ARPES data. The comparison with the literature has clarified the reliability of our analyses, which shows the emergence of prominent peak structures in the normal and anomalous parts of the self-energies and their

cancellation in the Green's function resulting in the direct invisibility in ARPES, while the prominent peak is the origin of the high temperature superconductivity [13]. The accuracy and reliability of the present machine learning method were confirmed by several benchmark tests, which successfully reproduced the expected exact results and the established analyses in the literature. It further established the robustness against unavoidable experimental noise and extrinsic contributions to spectral functions such as background effects. The origin of the failure of previous studies which did not find the prominent structure in the self-energies are exposed by faithfully following the assumptions by the previous studies and by showing the error contained in the assumptions.

More thorough studies of the integrated spectroscopy analysis have been conducted in the combination of ARPES, and QPI or RIXS. By using the ARPES data and their machine learning analyses, a two-component fermion model is constructed to represent the fractionalization of electrons supported by the previous theoretical and experimental studies. Then the two-component Hamiltonian was analyzed to predict the RIXS data [14]. The prediction shows a substantial enhancement of the RIXS intensity in the superconducting phase in comparison to the normal phase, if the electron fractionalization correctly describes the low energy dynamics of the cuprate superconductors. Since such an enhancement does not occur in the absence of the fractionalization, it can be used as the stringent test for the occurrence of the fractionalization.

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