Mechanism of pseudogap and superconductivity with low-energy fermionic excitations in high-T_c cuprates

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Recent progress in accuracy of numerical simulations has enabled much more precise determination of the ground states of the strongly correlated systems than before. Thanks to the progress, it has recently been elucidated how the *d*-wave superconducting and stripe states are severely competing in the simple Hubbard models by using combined variational Monte Carlo, tensor network and Lanczos methods [1,2] consistently with other methods. It has revealed that the ground states of most part of carrier doped Mott insulator in the Hubbard model are various periodicity of stripe states.

On the other hand, *ab initio* Hamiltonian of carrier doped $HgBa_2CuO_4$ recently derived without any adjustable parameters beyond model studies [3,4] by applying multi-scale *ab initio* scheme for correlated electrons (MACE) has been studied by applying the same improved numerical method [5], where the competition of stripe and superconductivity well reproduces the experimental phase diagram. More concretely, a high-T_c cuprate superconductor $HgBa_2CuO_{4+}$ has been studied by solving an *ab initio* low-energy effective Hamiltonian. Its ground-state phase diagram reproduces experiments including Mott gap, antiferromagnetic ordered moment in the mother material and superconducting phase extended in a wide range of hole density, which severely competes with a period-4 charge ordered state near $\delta \sim 0.1$ as is observed by recent X-ray scattering measurements. Crucial role of off-site interactions on the amplitude and stability of the superconductivity is revealed. Furthermore, we find that the enhancement of superconductivity is well correlated with that of charge fluctuations rather than spin fluctuations.

Based on the superconductivity reproduced by the numerics, we have also studied the superconducting mechanism in more depth. An experimental long-standing puzzle was the featureless structure in the spectral function indicated by the angle resolved photoemission spectroscopy (ARPES) spectra, in contrast to the case of conventional strong-coupling BCS superconductors in the history. We have shown before how the puzzle has been solved with the help of quantum-cluster studies of dynamical mean-field theory (DMFT) of the Hubbard model, where the featureless structure is a consequence of the cancellation of the prominent peaks in both of the normal anomalous part of self-energies [6,7].

We have recently examined this problem from a completely independent machine learning studies purely based on the ARPES data [8]. Recent progress of machine-learning techniques opens possibilities of exposing physical quantities hidden in direct measurements only from available experimental data combined with nonlinear regression analyses. The Boltzmann-machine method has been applied to the angle-resolved photoemission spectroscopy spectra of cuprate superconductors. The result shows that prominent peak structures exist both in normal and anomalous self-energies, but they cancel in the total self-energy making the structure apparently invisible, while the peaks make dominant contributions to superconducting gap, hence providing a decisive testimony for the origin of superconductivity. This is consistent with the former DMFT studies of the Hubbard model. The present achievement opens avenues for innovative machine-learning spectroscopy method. An emergent dark fermion theory has also been discussed in detail in connection to the peak structure revealed above [9].

We have further formulated a method of deriving effective low-energy Hamiltonian for nonperiodic systems such as interfaces for strongly correlated electron systems by extending MACE to make challenging studies of lattice relaxation around the interface possible. We have applied the formalism to copper-oxide high T_c superconductors in an example of the interface between overdoped $La_{2-x}Sr_xCuO_4$ and Mott insulating La_2CuO_4 recently realized experimentally [10]. We show that the parameters of the two-orbital *Eg* Hamiltonian derived for the $La_2CuO_4/La_{1:55}Sr_{0:45}CuO_4$ superlattice differ considerably from those for the bulk La_2CuO_4, particularly significant in the partially-screened Coulomb parameters and the level difference between the d_{x2-y2} and d_{z2} orbitals, ΔE. Here, the lattice relaxation on the E_g Hamiltonian has been examined from first principles. We find that the CuO_6 octahedra distort after the relaxation as a consequence of the Madelung potential difference between the insulator and metal sides, by which the layer dependence of the hopping and Coulomb parameters becomes more gradual than the unrelaxed case. Furthermore, the structure relaxation dramatically changes the ΔE value and the occupation number at the interface. This study not only evidences the importance of the ionic relaxation around interfaces but also provides a set of layer-dependent parameters of the *ab initio Eg* Hamiltonian, which is expected to provide further insight into the interfacial superconductivity when solved with low-energy solvers.

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