PCP6-1

Variational Monte Carlo Study of Excited States in Strongly Correlated Hubbard model

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In recent experimental research, excited states were artificially produced by irradiating various (doped) Mott insulators with pulsed light or by modulating the periodic potential of optical lattices in cold atom systems, and relaxation processes from them were actively studied. For example, it was discussed that when one excites parent compounds (antiferromagnetic Mott insulators) of cuprate superconductors, the features of metallization are different between the compounds for hole-doped and electron-doped systems [1]. So far, most theoretical studies have addressed dynamical relaxation processes, but it is also important to elucidate static properties of many-body excited states because they are not necessarily what are expected from the band theories. For example, how much doublon density, namely, light intensity is needed to make a Mott insulator metallic.

In this work, we study static properties in the initial quasi-steady states after an excitation beyond the Hubbard gap, by applying a variational Monte Carlo (VMC) method to a two-dimensional Hubbard model with diagonal transfer (t'). We can make a trial wave function for an initial excited state by regulating the lowest number of doublons D_L to $D_L>0$, legitimately at least in the Mott insulating regime; for the ground state, $D_L=0$. We primarily consider fundamental features of excited states at half filling for intermediate and strong correlations, for instance, the threshold of doublon density to metallize a Mott insulator as a function of U/t and t'/t [2] or how superconducting (SC) correlation is enhanced immediately below the Mott transition point U_c/t, as compared to the ground state. Secondly, how this SC correlation evolves as doping rate increases. In the presentation, we explain the details of formalism and discuss basic results.

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Keywords: excited state, cuprate superconductor, Mott transition, variational Monte Carlo method

PCP6-2

Model Constraction and Fluctuation Exchange Study of a New Cuprate Superconductor $Ba_2CuO_{3+\delta}$

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Despite a long history exceeding three decades, the high-T_c cuprate superconductors have basically the same essential ingredient, the CuO_2 plane. Typically, high-T_c cuprates have a layered perovskite structure, where the Cu-O octahedron is elongated along the c axis, so that the $3dx^2$-y^2 orbital is located at the top among the $3d$ bands. In a previous study[1], it was shown that the separation of the $3dx^2$-y^2 orbital from other (especially $3d3z^2$-r^2) orbitals plays an important role in realizing high T_c d-wave superconductivity. Therefore, a large apical O height should in general favor high T_c as far as the CuO_2 plane is concerned with about 15% hole doping being "optimal" for the highest T_c.

Recently, Li *et al.* [2] reported high-T_c superconductivity in a new cuprate $Ba_2CuO_{3+\delta}$ with a K_2NiF_4-like layered structure. There, they find several unique features which strongly suggest that the material is a different type of cuprate superconductor that opens up a new paradigm. Namely, a large amount of O vacancies are present within the CuO_2 planes, and a great amount of holes are doped which should cause a large deviation of the Cu valence from 2+. Also, the distance between Cu and the apical O is shorter than the in-plane Cu-O distance, so that the octahedron is compressed along the c axis. This should result in a crystal field where the $3d3z^2$-r^2 orbital is lifted in energy above the $3dx^2$-y^2 orbital. These findings suggest that the mechanism of superconductivity in the $Ba_2CuO_{3+\delta}$ may be considerably different from that for the conventional cuprates.

For the 2-1-3 composition in particular, the chain structure is known to be stable in an actual material Sr_2CuO_3. As another possibility within the 2-1-3 composition, here we consider a Lieb lattice type structure. First principles total-energy calculation performed with the VASP code shows that the chain and the Lieb lattice structures are close in the total energy, so that the latter may also be considered as a candidate. Focusing on these two structures, we construct multiorbital Hubbard models, and discuss the possibility of superconductivity within the fluctuation exchange approximation.

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[2] W. M. Li *et al.*, Proc. Natl. Acad. Sci. U.S.A. **116**, 12156 (2019).

Keywords: Cuprates, Theory, Ba2CuO3+δ, Lieb lattice

PCP6-3

Anisotropy in strongly correlated electrons and its relationship with superconductivity

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Recently, symmetry-breaking phenomena have been successively found in various superconductors; electronic nematic order breaking the rotational symmetry [1] and charge density wave breaking the translational symmetry [2] were experimentally discovered along with superconductivity (SC). Thus, it is urgent to clarify the relationship between these novel symmetry breaking phenomena and SC because they may provide important insights into the relationship between SC and the enigmatic pseudogap state. Pomeranchuk instability, a spontaneous breaking of four-fold rotational symmetry of the Fermi surface without lattice distortion, is a noteworthy candidate for the nematicity observed in cuprate superconductors [3].

In this presentation, we check whether an anisotropy spontaneously appears or not in strongly correlated electrons that have a complex phase diagram of SC and antiferromagnetism (AF). To this end, we use a variational Monte Carlo method (VMC) for the square-lattice Hubbard model with diagonal transfer t' and large U, and consider the relationship between the anisotropy and SC when the model parameters varied.

We introduce the following features in trial wave functions: (1) Band renormalization effect owing to electron correlation is introduced by adjusting the parameters of hopping integrals, some of which have degree of freedom of anisotropy in x and y directions. (2) As multi-body correlation factors, a doublon-holon binding factor and an on-site Gutzwiller factor are used to capture the essence of strong correlation.

First, we calculate the properties of pure SC, pure AF, and normal states individually by VMC method and consider what is the most important factor in Pomeranchuk instability by comparing the magnitude of x-y anisotropy. Next, we adopt a mixed state of AF and SC orders as a trial wave function, by which we can treat the orders continuously from their coexistence to the mutual exclusivity. With this wave function, we will clarify the relationship between anisotropy and SC or AF order in the strongly correlated regime.

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Keywords: Cuprate superconductor, Hubbard model, Nematicity, Pomeranchuk instability

PCP6-4

Study of Optical Properties in Triple-Layer Cuprate Bi2223

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$Bi_2Sr_2Ca_2Cu_3O_{10}$, "Bi2223", which is one of the multilayer cuprate superconductors, has three CuO_2 layers per unit cell. The optimally doped Bi2223 shows the superconductivity below T_c = 110K. Recently the superconducting gap in each layer has been determined by angle-resolved photoemission[1] and Raman scattering spectroscopy[2]. The observed gap sizes and the gap/T_c ratio were much larger than those of single- and double-layer cuprates.

Because of this relatively higher T_c and larger superconducting gap, it is expected that the change of the optical feature by superconducting transition appears at higher energy region and at higher temperatures above T_c. However, there has been so far no report of optical spectra of Bi2223 probably because of a lack of large crystals. In this work, we performed in-plane ($E \perp c$) optical reflectivity measurements by Fourier transform infrared (FTIR) spectroscopy in optimally doped Bi2223. We succeeded in observing a rise of reflectivity below T_c around 1000 cm^{-1}, suggesting the suppression of the optical conductivity with forming Cooper pairs.

[1] S. Ideta, *et al.*, Phys. Rev. Lett. **104**, 227001 (2017)
[2] G. Vincini, *et al.*, Phys. Rev. B **98**, 144503 (2019)

Keywords: High-Tc cuprate, Optical properties, Superconducting gap

PCP6-5

Simulation of THz emission from various shaped intrinsic Josephson junction arrays

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High-T_c cuprate superconductors have several special properties: higher superconducting transition temperature and unconventional Cooper pairing. Additionally, in these materials, superconducting layers and insulating layers are piled up alternately, thus the Josephson junctions between layers are formed spontaneously. These junctions are called the intrinsic Josephson junctions.

If a voltage is applied to the Josephson junctions, an ac current flows by the Josephson effect. Because of this ac current, this electromagnetic (EM) wave is emitted from junctions, and frequency of this wave reaches to the THz regime.

The frequency of the THz wave depends on the applied voltage, also the shape of the material. In some shapes, the EM wave have a circular polarization.

In this study, we simulate the EM field in the junction and the EM wave emitted to outside of the junction numerically using the finite element method and the boundary element method. In a junction array, we use the finite element method and solve Josephson relation considered coupling between the junctions [1], spatial variations of phase differences in magnetic wave,and the Maxwell equation.

And outside of the junctions, we obtain emitted EM wave by using the boundary element method. Then we investigate the dependence of the EM wave on the shape of the junction array.

[1] T. Koyama, H. Matsumoto, M. Machida, K. Kadowaki, Phys. Rev. B **79**, 104522 (2009)

Keywords: High-Tc cuprate superconductors, Intrinsic Josephson junctions, THz emission, Finite element methid

PCP6-6

Exotic Properties of High Temperature Cuprates Superconductor

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In spite of much interest in various exotic properties of superconducting cuprates such as the pseudogap, strange metal in normal state, anomalies in the optical sum rules, and several exotic phases of the electron-nematic order *etc* [1], its microscopic mechanism still remains unsolved issues. Here these properties are considered using our recently proposed theory emphasizing that the electronic state of superconductors can be described by the composed fermions [2,3,4]. It is found that the anisotropic pseudogap can be derived from pseudogap state with the representation in momentum space, and that T-linearity of the electrical resistivity in optimal doping can be derived from considering the interplay between the composite fermion bands. It is also found that the anomaly of optical sum rules can be explained in a similar mechanism.

[1] B. Keimer *et al.* Nature **518** (2015) 179.
[2] K. Nishi, J. Phys. Conf. Ser. **871** (2017) 012033.
[3] K. Nishi, J. Phys. Conf. Ser. **1054** (2018) 012013.
[4] K. Nishi, Phys. Lett. A **382** (2018) 3293.

Keywords: high temperature superconductor, cuprates, exotic properties

PCP6-7

Superconductivity in the heavily Pb-doped Bi-2212 phase of $(Bi,Pb)_2Sr_2CaCu_2O_{8-\delta}$

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The superconducting transition temperature T_c of the Bi-2212 phase of $Bi_2Sr_2CaCu_2O_{8+\delta}$ is ~ 80 K. The reason of the relatively low T_c is that the hole-concentration is situated in the overdoped region because extra oxygen atoms easily introduced in the BiO plane supply the CuO_2 plane with holes excessively. The structural disorder caused by extra oxygen atoms also suppresses superconductivity. Recently, we have succeeded in increasing T_c up to 102 K in $Bi_{1.64}Pb_{0.36}Sr_2CaCu_2O_8$ by the optimization of the content of Pb^{2+}-substitution for Bi^{3+} and the complete removal of extra oxygen atoms through the reduction annealing [1]. With further increasing Pb-content, it is expected that the oxygen deficiency occurs. In this study, we have investigated the effects of the oxygen deficiency on T_c in the heavily Pb-doped Bi-2212 phase of $(Bi,Pb)_2Sr_2CaCu_2O_{8-\delta}$.

Polycrystalline samples of $Bi_{2-x}Pb_xSr_2CaCu_2O_{8-\delta}$ ($0 \le x(Pb) \le 1$) were prepared by the solid-state reaction method and annealed in flowing gas of Ar in the final step to suppress the formation of impurity phases with Pb^{4+}. As shown in Fig. 1, almost single-phase samples can be obtained for $x(Pb) \le 0.6$ through the Ar-annealing at 710-750°C. As for $x(Pb) = 0.8$, almost single-phase sample is obtained through the Ar-annealing at 730°C. We will report the effects of the oxygen deficiency on T_c.

[1] K. Sugawara *et al.*, J. Phys.: Conf. Ser. **1054** (2018) 012008.

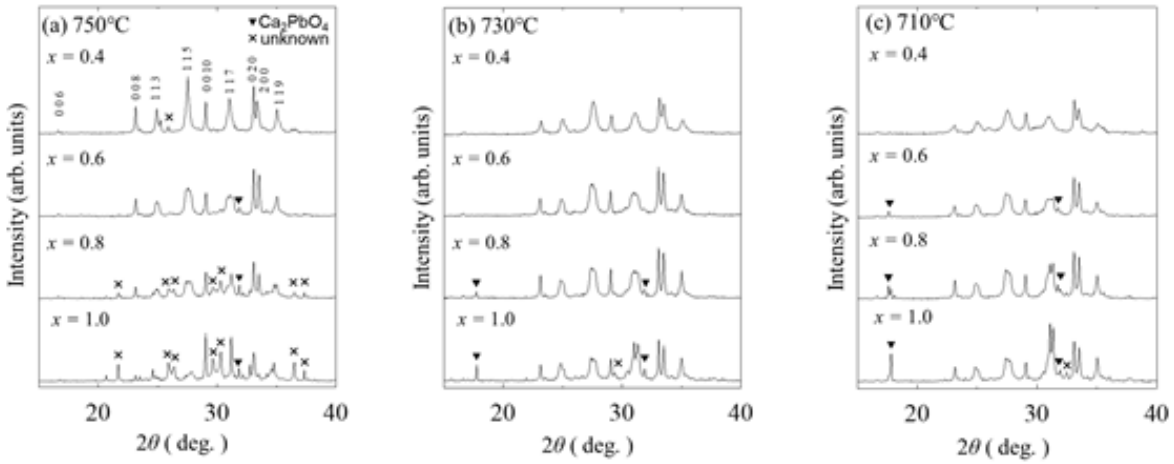

Fig.1. Powder X-ray diffraction patterns of $Bi_{2-x}Pb_xSr_2CaCu_2O_8$ ($0.4 \le x(Pb) \le 1$) obtained after the Ar-annealing at (a)750°C, (b)730°C and (c)710°C.

Keywords: Bi-2212, Pb-substitution, Oxygen deficiency