PCP6-1

Phase Diagram of High-Temperature Superconducting Cuprates and Iron Pnictides

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Phase diagram of high-temperature superconducting cuprates and iron pnictides is considered based on the theory emphasizing that the electronic state of superconductors can be described by the composed fermions. The theory is constructed with the Hamiltonian which is so modified by the unitary transformation using these fermion operators as to apply the mean field approximation [1]. The ground and excited states of the Hamiltonian are calculated using two representations in real and momentum space. The doping dependency of the gap energy, critical temperature and band structure *etc* are evaluated in various states such as pseudogap and superconductive states. It is indicated that the phase diagram about superconducting and non-superconducting states of cuprates and pnictides can be explained from the viewpoint of unifying two types of these superconductors.

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Keywords: High-temperature superconductivity

PCP6-2

An Analysis of high-T_c cuprates in the superconducting state incorporating strong correlation effects based on a self-consistent perturbation expantion

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Many theoretical studies have been performed to describe basic properties of high-T_c superconductors. Noteworthy among them is the fluctuation exchange (FLEX) approximation [1]. This formulation incorporates higher-order terms in the perturbation expansion self-consistently satisfying conservation laws simultaneously. The FLEX approximation have been successful in reproducing various in normal-state properties of high-T_c superconductors, especially transport phenomena. However, the standard FLEX approximation cannot describe superconducting properties. Moreover, some approaches for the superconducting state don't satisfy the conservation laws, so we can't describe the transport phenomena appropriately. Recently, a consise extension of the FLEX approximation to the superconducting state was developed, called FLEX-S approximation [2]. This extention was performed by incorporating all the pair process by symmetrizing the vertex of each Feynman diagram considered in the original FLEX approximation. Using this formulation, we can perform a self-consistent perturbation expansion. This approach is expected to describe the properties of the superconducting state in such a way as to extend the FLEX approximation for the normal state. Note in this context that these two formulations satisfy various conservation laws naturally. In this presentation, we report calculations of the spectral function and the density of state in superconducting state based on the FLEX-S approximation. In this calculation, we apply this formulation to the Hubbard model on a 2D square lattice assuming a spin-singlet pairing. We set the parameters in the Hubbard model so as to reproduce the observed band structure of cuprate superconductors [3]. We show the band structure, the Fermi surface, the ralaxation time of the quasiparticle estimated by the spectral function, and the pair potential.

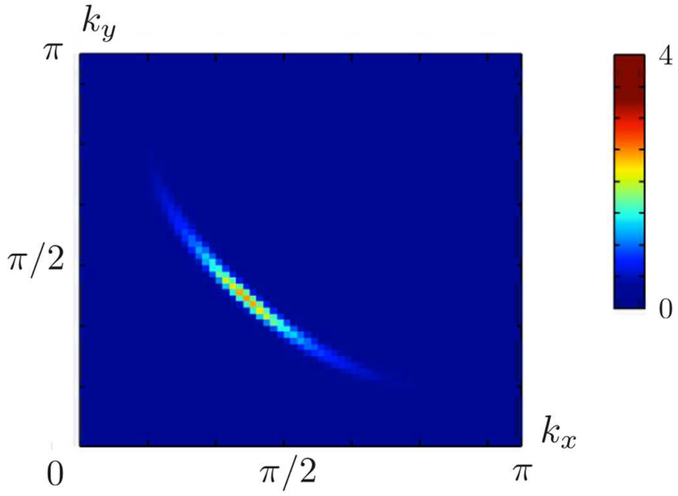

Fig.1 The Fermi surface of the YBCO model. We can see Fermi arc near k_x~k_y

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Keywords: high-Tc superconductor, self-consistent perturbation expansion, FLEX-S approximation

PCP6-3

Impurity-induced Mott transition in Doped Hubbard model

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Recent numerical studies [1] on the two-dimensional Hubbard (t-t'-U) model argued that antiferromagnetic (AF) (or phase-separated) states, instead of superconducting states, prevail up to $\delta \sim 0.2$ of doping rate for any t'/t. This result obviously contradicts the experiments of cuprate superconductors. For reconciling this contradiction, we have been studying the effects of point-type impurity potentials inherent in cuprates on paramagnetic (PM) and the AF states by means of a variational Monte Carlo (VMC) method. In a preceding publication [2], we argued that an impurity potential V of $U \lesssim V < V_{\rm M}$ with $V_{\rm M}/t \sim 2$ (U/t=12), namely in attractive and weakly repulsive cases, is almost screened out for strong correlations ($U/t \gtrsim 8$). As a result, the properties of the PM and AF states for the uniform case (V=0) are preserved in this range of V; for example, the AF states are metallic with pocket Fermi surfaces, whose positions depend on whether $t' > t_{\rm L}$ [~(π,0), type I] or $t' < t_{\rm L}$ [~(π/2,π/2), type II] with $t_{\rm L}/t \sim 0.05$ (U/t=12).

In this presentation, we focus on the regime of repulsive potentials (V>0), which are realistic to cuprates. For $V > V_{\rm M}$, the optimization in our VMC calculations does not converge in the PM state and has large fluctuations in the AF state. In this regime of V, staggered magnetization becomes large, especially, for the impurity density of $\delta_{\rm imp} \geq \delta$. We find that the AF state with $\delta_{\rm imp} \geq \delta$ is gapped by analyzing the momentum distribution function $n(\mathbf{k})$---the pocket Fermi surfaces vanish. Furthermore, the electron density in ordinary (non-impurity) sites is found to be preserved at 1 (half filling) for any $\delta_{\rm imp}$ ($\geq \delta$), by adjusting the electron density in impurity sites. It indicates that an impurity-induced Mott transition takes place at $V = V_{\rm M}$ in the AF state.

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Keywords: cuprate, antiferromagnetic state, impurity potential, Mott transition

PCP6-4

Interhole correlation and Phase Separation in *t-J* model

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In connection with cuprate superconductors, it is important in the *t-J* model on the square lattice to clarify at what values of *J/t* the correlation between holes is switched from repulsive to attractive ($J_{\rm I}/t$) and phase separation takes place ($J_{\rm PS}/t$) [1] for a specific values δ (doping rate). In the limit of $\delta\rightarrow 1$, it is exactly known that $J_{\rm I}/t$=2 [2] and $J_{\rm PS}/t$ =3.4367 [3], whereas for small values of δ of our interest, the problems---for instance, how $J_{\rm I}/t$ and $J_{\rm PS}/t$ evolves as δ decreases---are still unestablished. Some researchers seem to consider that the correlation is attractive even for $J/t\sim$ 0.3, a plausible value for cuprates.

In this study, we reconsider these problems using a many-body variation theory with recently developed wave functions and procedures. In the limit of $J/t\rightarrow 0$, total energy (E/t) is lowered only by the hopping (t) term, so that the correlation should be repulsive in order to keep other holes away and the state should be uniform (not phase separated). On the other hand for $J/t\rightarrow\infty$, E/t is reduced only by the superexchange (J) term. Thus, the correlation should be attractive and the state phase separates. Because the values of $J_{\rm I}/t$ and $J_{\rm PS}/t$ depend on δ, first we fix J/t at 0.3 and study properties of the states with *d*-wave superconducting (*d*-SC) and antiferromagnetic (AF) orders for some values of δ. Then, we consider J/t dependence.

In estimating expectation values, a variational Monte Carlo method is employed for Jastrow-type wave functions. As a many-body factor, we use a long-range Jastrow factor, because hole pairs of long distance come to play an appreciable role as δ increases. In the one-body part, we use mixed wave functions of AF and *d*-SC orders, in which band renor- malization effects are introduced [4]. We also make a comparison with related studies [5].

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Keywords: t-J model, interhole correlation, phase separation, variational Monte Carlo

PCP6-5

Interplay between Staggered Flux and *d*-Wave Superconducting Orders in *t*-*t'*-*J* Model

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To understand the superconductivity (SC) in high-T_c cuprates, it is important to find out the origin of pseudogap phenomena, which behave like a shadow of SC [1]. Some experiments reported coexistence of the pseudogap and a SC gap [2]. Among various candidates for the pseudogap state, a staggered flux (SF) state, characterized by local circular currents in plaquettes that flow clockwise and counterclockwise alternately, was confirmed to be moderately stable and have properties mostly consistent with the pseudogap behavior [3]. In a previous publication [4], we studied whether the *d*-wave superconducting (*d*-SC) order coexists with or excludes the SF order, by applying a variational Monte Carlo (VMC) method to the square-lattice Hubbard (*t*-*t'*-*U*) model with diagonal transfer *t'*. It is found that the SF order competes with the *d*-SC order and is never stabilized for $U/t=12$ regardless of t'/t.

In this presentation, we consider the same issue for the *t*-*t'*-*J* model obtained from the strong coupling expansion of the Hubbard model. We check again whether the SF order coexists with or is excluded by the *d*-SC order, to compare with the previous result for the Hubbard model. In the trial wave function, we introduce the following features:

(1) We allow for the coexistence of SF and *d*-SC orders, by which we can treat a continuous description of their interplay from mutual exclusivity to coexistence.

(2) Inter-site S_z-S_z spin correlation factor is introduced in addition to the ordinary Jastrow correlations.

(3) Band renormalization effects are considered by adjusting the parameters of hopping integrals up to the fifth-neighbor sites; these effects are important near half filling.

In addition to clarifying the difference between the two models, it is interesting to discuss differences between the results of variationally accurate VMC methods and of Gutzwiller (mean-field-type) approximations [5].

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[5] H. Tsuchiura, unpublished; M. Ogata, unpublished.

Keywords: Cuprate, Pseudogap, Staggered flux, t-J model

PCP6-6

Effects of Diagonal Hopping on Loop Currents in Fermionic Hubbard Model

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States with loop-current orders have been theoretically discussed as the origin of the pseudogap in cuprate superconductors, because the loop currents break time reversal and other symmetries [1,2] as some experiments observed below T^*. In addition, bosonic-Hubbard models with magnetic fluxes along a certain direction were virtually realized in ultracold-atom systems [3]. Thus, it is urgent to clarify the properties of loop-current states in a fermionic-Hubbard model with a magnetic flux. In such a background, we began to study a staggered-flux (ST) order which is a kind of loop-current orders [4], by means of a variational Monte Carlo method.

In the preceding study, to study the influence of a magnetic order on loop currents, we introduced a mixed state of ST and antiferromagnetic (AF) orders on the square lattice without diagonal hopping ($t'=0$). We found in non-doped (half-filled) cases that the two orders coexist for a finite magnetic flux, and the AF order increase the loop currents in a Mott insulator phase, whereas a state with a pure AF order is stabilized without a magnetic flux. In another recent study regarding a coexistent state of d-wave superconducting (d-SC) and AF orders [5] reported for doped systems that as t' is increased, the locus of Fermi surface in a pure AF state switches from around (π/2, π/2) to around (π, 0) at $t'=t_L\sim-0.05t$, and that this change is crucial for the appearance of a coexistent state.

Here, we study how diagonal hopping t' influences a mixed state of AF and ST orders in the Hubbard (t-t'-U) model. Recall that the pure ST state becomes metallic in doped cases with a Fermi-arc-like Fermi surface centered at (π/2, π/2) regardless of t', and this pocket Fermi surface is topologically the same as (in discord with) that of the pure AF state for $t'<t$L ($t'>t_L$), as above. It is indispensable for treating t' dependence to introduce band renormalization effects [5] in the AF part of a trial wave function. In the presentation, we would like to also consider band renormalization effects in the ST part.

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Keywords: staggered flux, antiferromagnetism, coexistent state, cuprate

PCP6-7

Optimized wave function by kinetic renormalization effect in strongly correlated region of the three-band d-p model for cuprate superconductors

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The mechanism of high-temperature superconductivity has been studied intensively since the discovery of cuprate high-temperature superconductors. It is certain that the electron correlation plays an important role in cuprate superconductors because parent compounds without doped carriers are insulators. It is important to clarify the phase diagram of electronic states in the CuO_2 plane. We investigate the ground state of the strongly correlated electronic models by employing the variational Monte Carlo method. We consider the three-band d-p model as well as the two-dimensional Hubbard model. We use the improved wave function that takes into account inter-site electron correlation beyond the Gutzwiller wave function. The ground-state energy is lowered considerably, which gives the best estimate of the ground-state energy for the two-dimensional Hubbard model in the world. We argue that there is a crossover from weakly to strongly correlated regions as the on-site Coulomb repulsion U increases when holes are doped. The antiferromagnetic (AF) correlation function increases as U increases in weakly correlated region, and has a peak at the intermediate value of U which is of the order of the bandwidth. The large U, greater than the bandwidth, suppresses the AF correlation to lower the ground-state energy by obtaining the kinetic energy gain. The large spin and charge fluctuations are induced in the strongly correlated region. This results in electron pairing and would lead to high-temperature superconductivity. The conventional spin fluctuation in weakly correlated region should be distinguished from that in strongly correlated region. It is just the spin fluctuation in strongly correlated region that would induce high-temperature superconductivity.

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Keywords: electron correlation, high-temperature superconductivity, optimized wave function, mechanism of superconductivity