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Project Progress Report

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Within this year, we concentrate mainly on the problems in high T_c cuprates: in particular, comparison between results of variational wave functions (VWFs) and observation by angle-resolved photoemission spectroscopy (ARPES) and scanning tunneling spectroscopy (STS). Results have been presented in two international conferences, as mentioned below, and will all be summarized in a written form soon. In the following, we discuss some of them in more detail.

(I)VWF versus ARPES results:

With the input from ARPES experiments completed recently by people in groups of A. Fujimori (University of Tokyo) and Z.-X. Shen (Stanford University), we extracted the Fermi surface properties of the VWF- resonating valence bond (RVB) WF for the extended *t-J* model (including long-ranged hopping *t'* and *t"*). Some of our VWF results are shown in figures at the end of this report and discussed below. The VWF work is in collaboration with Mr. Chun-Pin Chou (National Tsing Hua University; Academia Sinica), Profs. C.T. Shih (Tunghai University) and T.K. Lee (Academia Sinica).

With the much improved momentum and energy resolution, the present ARPES can map out quite accurately the whole Fermi surface (FS) which may be compared with the quantities observed in thermodynamic experiments. Especially, the FS evolution with hole doping in $La_{2-x}Sr_xCuO_4$ (LSCO) [1] and $Bi_2Sr_{2-x}La_xCaCu_2O_{8-y}$ (Bi2212) [2] has been carefully studied. The (0,0)-to-(π,π) or nodal FS position, FS shape or topology and the extracted density of states (DOS) have been shown to have contrasting behaviors in these two materials [2].

We applied the VWF approach to examine whether this behavior can be understood in terms of the RVB WF. The different materials turn out to be characterized by different hopping parameter sets of (*t'/t, t"/t*) [=(*-0.3, 0.2*) and so on] typical for real materials in the *t-t'-t"-J* model. Recognizing that, as the density of doped holes in the models is increased, the WF described above is switched from the one with explicit antiferromagnetic ordering, but negligible *d*-wave superconducting pairing [3] to those with finite pairing amplitudes of charge carriers [4], we focus on the latter ones which also have the large FS (instead of the "Fermi pockets" for WFs at low doping [3]). We examine here the original *d*-wave RVB (*d*-RVB) WF

$$|RVB\rangle = P_d \prod_k u_k + v_k c^+_{k\uparrow} c^+_{-k\downarrow} |0\rangle$$

with the usual coherent factor $[\mathrm{k}=(k_x,k_y)]$ $v_\mathrm{k}/u_\mathrm{k}=\Delta_\mathrm{k}/(\varepsilon_\mathrm{k}+\sqrt{\varepsilon_\mathrm{k}^2+\Delta_\mathrm{k}^2})$ where the *d*-wave pairing amplitude $\Delta_\mathrm{k}=\Delta(\cos k_x-\cos k_y)$ and the electron dispersion $\varepsilon_\mathrm{k}=-2t(\cos k_x+\cos k_y)-4t'\cos k_x\cos k_y-2t''(\cos 2k_x+\cos 2k_y)-\mu$. The operator P_d enforces the constraint of no double occupancy. For hopping parameters (*t'/t, t''/t*) =(*-0.3, 0.2*), as the hole concentration is in the optimal (*x~0.3*) and overdoped regions the pairing (by computing the pair-pair correlation in the fixed-particle representation of the VWF [4]) is greatly enhanced. The pairing strength is less enhanced for smaller values of (*t'/t, t''/t*) =(*-0.1, 0.05*) and the optimal doping position is around *x~0.20*. This contrast is then argued to be related to the different topologies (and thus different evolution behaviors with doping) of the Fermi surface for different hopping amplitudes [4]. Compare with the experiments, we intend to consider carriers in LSCO to have small hopping strength, in contrast to the larger values (and thus higher *Tc*) associated with Bi2212.

Focusing on the doping evolution of electronic states observed in ARPES, we have calculated the quasi-hole excitation spectrum of the optimized *d*-RVB WF by adding one extra hole for doping levels we studied. Main results are shown in the figures attached at the end of this report.

Fig. 1 (a)-(c) show the fitted quasi-hole dispersions $\varepsilon_\mathrm{k}^\mathrm{VAR}$ (by taking the pairing amplitude Δ_k to be zero) for excitation energies [*e.g.* Fig.1(a) is for the case of adding one extra hole in the system of size 12×12 with 12 holes originally.] at various doping levels with (*t'/t, t''/t*) =(*-0.1, 0.05*). Doping dependence of the FS position can then be examined as zero energy contour are extracted. Consistent with the FS positions observed in ARPES [1,2], the FS in the nodal direction, as shown Fig.2, moves slowly as doping is increased (as indicated by the dashed arrow). Fig.3 shows the similar doping dependence for the case with (*t'/t, t''/t*) =(*-0.3, 0.2*). The more prominent movement of FS position in the nodal direction than the previous is indeed seen in recent ARPES study on Bi2212 [2].

It is then straightforward to find the DOS for each doping by counting the number of states enclosed within the FS. The results are shown in Fig.4 for the case of (*t'/t, t''/t*) =(*-0.1, 0.05*). The area (in the unit of π^2) as a function of doping is shown in Fig.5. It is found to follow the "Luttinger sum rule", $(1-\delta)$, with doping δ. This is also consistent with the observation in LSCO by ARPES.

With the correspondence we found between VMC and ARPES results that the larger value of (*t'/t, t''/t*) is for the Bi2212 and the smaller (*t'/t, t''/t*) for the LSCO, we are now trying to understand the puzzles remained to be solved. The main question we are concentrating is whether the superconducting state solely the Bardeen-Cooper-Schrieffer (BCS) state with *d*-wave pairing symmetry but no features at all of the strong electron-electron interactions. One intriguing feature found in the analysis on FS properties for (*t'/t, t''/t*) =(*-0.3, 0.2*) case is the violation of the "sum rule". The experimental situation seems not to be settled due to the difficulty of determining the FS position near the anti-nodal or $(\pi,0)$ and $(0,\pi)$ regions. We are also working on systems with anisotropic hopping amplitudes which should help to understand the recent results on the ratio of *d*- and *s*-wave pairing amplitude in $YBa_2Cu_3O_7$ due to the particular (orthorhombic) lattice structure at low temperature. It is possible that the pairing strength directly due to the hopping and thus the band structure may not be able to account for the observed values. Instead, within the framework of *t-J*-models with strong correlations explicitly included, much enhancement of aniotropic pairing amplitude may be obtained in terms of the superexchange $J_{x(y)} \propto t^2_{x(y)}/U$ where U is the on-site repulsion. With this, we may provide a resolution to the relation between the superconductivity and strong electron correlations in these systems.

Part of the results have been presented in "The 4th International Workshop on Novel Quantum Phenomena in Transition Metal Oxides and The 3rd Asia-Pacific Workshop on Strongly Correlated Electron Systems" held in Sendai, Japan last November.

(II) Understanding the recent STS on cuprates:

To understanding further the nature of the superconducting state in cuprates, we have been concerning about phenomena seen in the STS which provides supplementary information for the electronic states. While ARPES probes, in short, the spectral function $A(\mathrm{k},\omega)$, the STS, by measuring the derivative of the tunneling current, *dI/dV*, at each position, **r**, probes the properties of the same fuction in real space [5], *i.e.*

$A_\mathrm{s}(\mathrm{r},\omega) = \sum_m \langle 0|c^+_\mathrm{r}|m\rangle\langle m|c_0^\beta|0\rangle\delta(\omega + E_m - E_0) + \sum_m \langle 0|c_\mathrm{r}|m\rangle\langle m|c_0^\dagger|0\rangle\delta(\omega - E_m + E_0)$, where $|0\rangle$ is the ground state of the system at some particular doping. Recent STS results have shown us that there are all varieties of phenomena existed in all high *Tc* cuprates properly studied- *e.g.* inhomogeneous distribution of gaps (inbetween the tunneling peaks) [6] and quasi-particle scattering at low energy in Bi2212 [7], patterns in *dI/dV* at low sample bias in $Ca_{2-x}Na_xCu_2OCl_2$ [8], asymmetry of *dI/dV* at positive (electron injected) and negative (hole injected) bias [], and so on.

Motivated by the recent theoretical work on the issue of tunneling asymmetry at positive and negative sample bias by Anderson and Ong [9] and Fukushima *et al.* [10]., we have been studying the properties of the spectral function near only the *d*-wave nodes at which the VWF approach may be applied. More precisely, we examine the matrix elements $|\langle\Psi_{N+1}|c^+_\mathrm{k}|\Psi_N\rangle|^2/[\langle\Psi_{N+1}|\Psi_{N+1}\rangle\langle\Psi_N|\Psi_N\rangle]$ and $|\langle\Psi_{N-1}|c_\mathrm{k}|\Psi_N\rangle|^2/[\langle\Psi_{N-1}|\Psi_{N-1}\rangle\langle\Psi_N|\Psi_N\rangle]$ which correspond to the positive and negative sample biased case, respectively, where $c^+_\mathrm{k}|\Psi_N\rangle$ is the quasi-particle and $c_\mathrm{k}|\Psi_N\rangle$ quasi-hole excited states from our ground states. Two strategies we have been using are discussed as follows.

(1) In collaboration with Prof. M. Ogata (University of Tokyo), we follow the proposal by Anderson and Ong to treat this issue by the Gutzwiller projection approximation. This approximation scheme employs explicitly the approach put forward by Laughlin recently to examine analytically the (partial) projection of non-double occupancy on the BCS state [11]. To keep the electron density the same as the projection strength is varied, a parameter called fugacity factor is included in the constructed WF. Turning on the projection, the *d*-wave superconducting state is associated with only a tiny superfluid density near half-filling (or zero doping) due to the on-site repulsion- thus called "gossamer" superconductivity (gSC). Intriguingly, there exists quasi-particle state of the gSC pinned within the “Hubbard-like” charge gap.

We focus here, in parallel with the study on other issues related to gSC, to calculate the matrix elements mentioned above as a function of the parameter of characterizing the projection strength. We may also examine the results by applying the extended Gutzwiller approximation scheme developed by Ogata and Himeda [12] in which the “off-site” mean-fields $\chi = \left\langle c_{i\sigma}^{+} c_{j\sigma} \right\rangle_0$ and $\Delta = \left\langle c_{i\uparrow}^{+} c_{j\downarrow}^{+} \right\rangle_0$, where i , j are nearest-neighbor sites and $\sigma(=\uparrow,\downarrow)$ represents spin index, are included in the *t-J* model case.

(2) The matrix elements with respect to the RVB state can be obtained straight numerically with the projection completely taken into account, even though only on finite lattices. To do this, we extend the quasi-hole states for studying the FS evolution with doping to the quasi-particle ones and calculate, with the associated normalization factors included, the overlapping with the ground states for *N-1* and *N+1* electrons, respectively. Cases for different doping and for lattices of different size are to be studied. We would hope to compare with the approximated results following strategy (1) and those by Fukushima *et al.* [10] which seems to show symmetric results for hole and electron tunneling.

In this variatioanl Monte Carlo study, I am collaborating with Prof. T.K. Lee (Academia Sinica) and his student Mr. Chun-Pin Chou (Natioanl Tsing Hua University and Academia Sinica). My two undergraduate-student assistants have been sorting out the basic theoretical formulation of the tunneling experiments with me.

We would hope to conclude this work by the end of this September.

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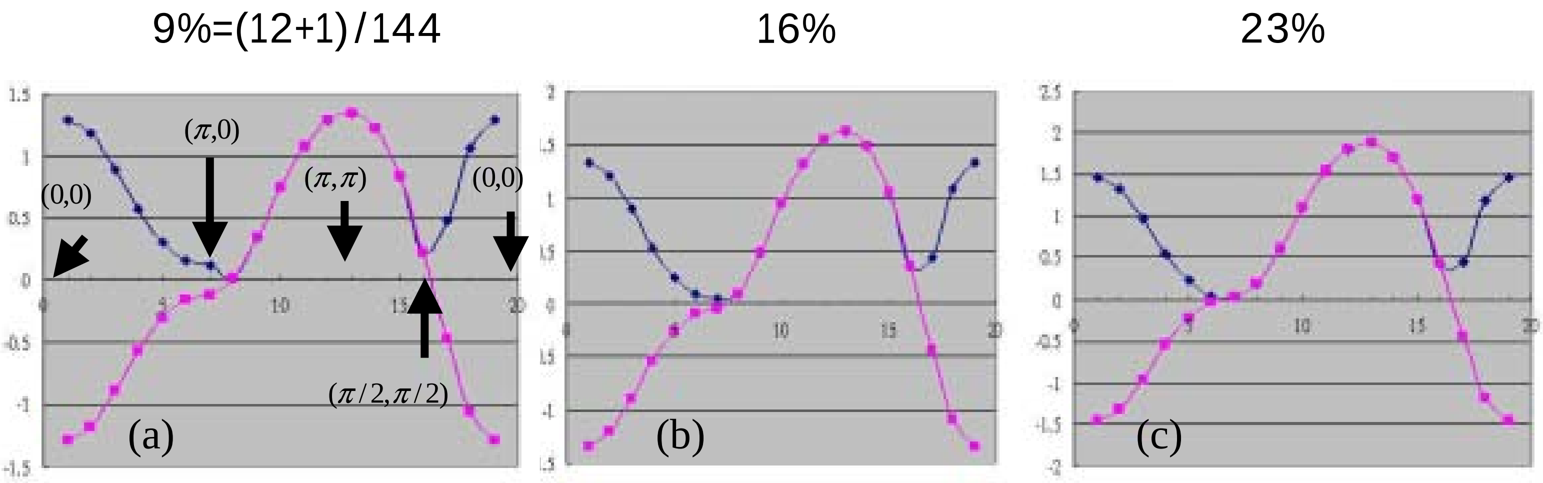

Fig.1

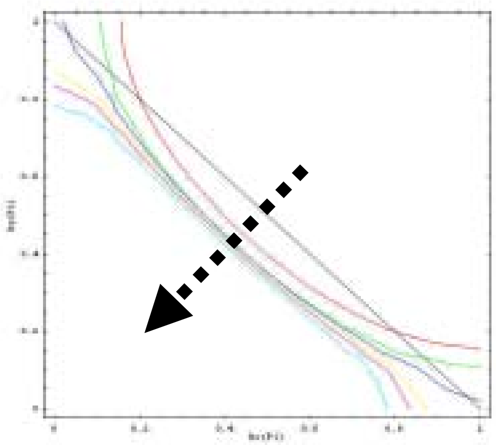

Fig.2

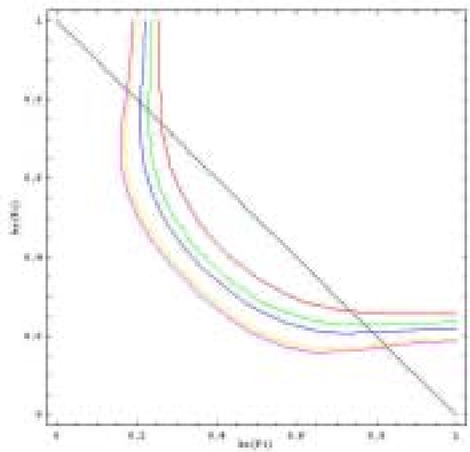

Fig.3

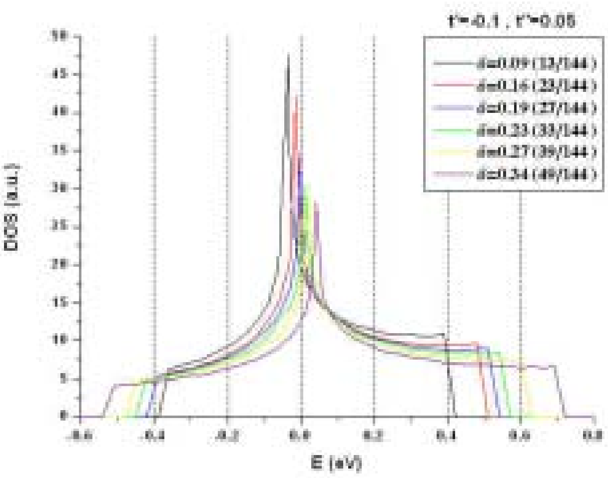

Fig.4

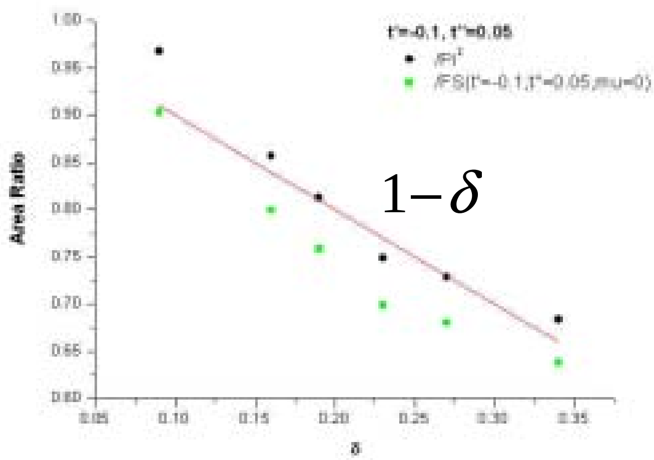

Fig.5