Single-Particle Spectrum in the Electron-Doped Cuprates

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We study the evolution of the single-particle spectrum with electron doping in a scheme which adds multiple exchange of transverse spin excitations to the mean-field antiferromagnetic insulator. Away from half-filling small Fermi surface pockets appear first around the X-points, and simultaneously new spectral weight grows in the insulating gap. With further doping the in-gap states develop the character of a renormalized quasiparticle band near the chemical potential. The essential features in momentum-energy space agree well with recent studies using angle-resolved photoemission spectroscopy on electron-doped cuprates. We interpret the origins and the nature of the in-gap states using a simple variational wavefunction.

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Recent angle-resolved photoemission spectroscopy (ARPES) experiments have determined the evolution of the Fermi surface in electron-doped cuprates, Nd$_{2−x}$Ce$_x$CuO$_{4+δ}$ [1]. In contrast to the hole-doped case, small Fermi surface pockets appear first near the X-points and then with further doping still in the presence of antiferromagnetic (AF) order, in-gap states appear around the zone diagonals with the character of renormalized band pockets. A further increase in doping leads to the formation of a single large Fermi surface. Note that ARPES for electron doping is more informative than for hole doping since the evolution of the charge-transfer gap [2]−[4] and discuss the physical origins of the in-gap states.

The ARPES experiments give clear evidence for electron-hole asymmetry, in agreement with the significantly different behavior of electron- and hole-doped cuprates [1, 2]. Similar contrasting behavior was found in recent one-loop renormalization-group studies [5]. A clear separation in energy scale between AF and superconducting fluctuations appears for electron-doping [5–7]. This explains the robustness of the AF phase [6] and the small doping range of the superconducting phase. For this reason, electron-doped cuprates can be treated as doped antiferromagnets within a coupling weak to moderate scheme, in contrast to hole-doped cuprates, where the AF fluctuations compete with the superconducting fluctuations leading to a crossover at relatively high energy scale to a strong coupling phase where all play a role [5–7, 8–10]. Strong coupling approaches give strong asymmetry [11] but the narrow region of the AF order upon hole doping greatly limits the approach we use here which starts from the AF mean-field (MF) state.

Since the AF Mott insulating state may be adiabatically connected to the MF-AF state at $T = 0$, the MF-AF state can be a good starting point for our purpose [12, 13, 14]. In order to take account of the collective spin-wave excitations (and also the particle-hole continuum), we calculate the single-particle self-energy including multiple exchange of RPA-type transverse spin excitations, i.e., so-called self-consistent Born approximation (SCBA) [15, 16]. Within this approach we can demonstrate the following. Away from half-filling small Fermi surface pockets occur first around the X-points, and simultaneously new spectral weight appears in the insulating gap. With further doping the in-gap states acquire the features of a renormalized quasiparticle band showing clear resemblance to that in the paramagnetic phase. To explain the physical origin of the in-gap state we introduce a simple variational wavefunction for the in-gap state, in which the quasihole MF state in the lower band admixes strongly with the hole state accompanied by particle-hole spin excitations in the upper band.

We work with the $t$-$t'$-$U$ Hubbard model,

$$H = \sum_{kσ} ε_k c_{kσ}^† c_{kσ} + U \sum_i n_{i↑} n_{i↓},$$

with a next-nearest-neighbor tight-binding dispersion:

$$ε_k = -2t (\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y,$$

where the lattice spacing $a = 1$. Throughout this paper, we set $t'/t = −0.3$ and $U/t = 8$. The outline of the SCBA calculation is as follows. First, we solve the AF-MF equation to determine the MF gap $Δ_0$ and the MF chemical potential $μ_0$ for a given electron density $n$.

$$1 \over U = 1 \over N \sum_k \sum_{σ} μ_0 + 2E_k-mE_k^0,$$

$$n = \sum_k \sum_{σ} μ_0 + E_k^0 \theta(μ_0-E_k),$$

where the MF-quasiparticle energy in the upper (lower) band, $m = +1(−1)$, is given by $E_{kσ} = ɛ_k + mE_k^0$, where $ɛ_k^± = (ɛ_k + Q ± ɛ_k)/2$ and $E_k^0 = \sqrt{(ɛ_k)^2 + Δ_0^2}$. Here $N$ is the number of sites and the summation of $k$ is taken over the magnetic Brillouin zone (MBZ). Note that the AF long-range order is always present in the doping range.
we study in this paper. We set up the RPA transverse susceptibilities (for normal and umklapp processes) using \( \Delta_0 \) and \( \mu_0 \), and solve the Dyson equation for the retarded Green’s functions at \( T = 0 \) putting these RPA susceptibilities into the one-loop self-energy. The true chemical potential, \( \mu \), is determined by \( n = 2 \int_{-\infty}^{\mu} d\omega \rho(\omega) \), where \( \rho(\omega) \) is the single-particle density of states (DOS) calculated from the resultant Green’s function. We discretize the momentum by \( 32 \times 32 \) mesh in the first quadrant and the energy by \( 1024 \) mesh in the interval \((-20t, 20t)\). Due to the omission of vertex corrections, the coupling constant in the self energy is too strong, which overestimates renormalization of the indirect gap \([15, 16]\). As shown by Bulut et al. \([17]\), a reduction of the coupling constant \( U \) mimics the effect of vertex corrections. We obtain a reasonable value of the indirect gap at half-filling with the reduced coupling constant, \( 0.7U \), in the self energy.

Figure 1 shows the doping dependence of the DOS. At half-filling \( n = 1.00^+ \) (with appropriate shift of the chemical potential to the bottom of the upper band), the multiple scattering by spin fluctuations redistributes the MF-quasiparticle weight into the incoherent background in an energy range \( \sim 8t \) accompanied by sharp quasiparticle peaks at the edges of the insulating gap. Based on the argument similar to Kane et al. for the \( t-J \) model \([18]\), we can conclude that the quasiparticle residue and its width are the order of \( t/U \) and \( 4t^2/U \), respectively. The intensity of the incoherent background is considerably enhanced at \( \omega - \mu \sim -7t \) and \( 3t \), which results from the coupling of the quasiparticle to interband particle-hole excitations across the gap \([18, 19]\).

With increasing electron doping, the position of the lower band moves down to lower energy with considerable reduction of the spectral weight. The reduction of the spectral weight, particularly in the lower band, leads to a transfer into the insulating gap giving rise to the in-gap states at \( \omega - \mu \sim -t \). As the doping increases further the in-gap states gain more spectral weight. Note that the chemical potential lies in the upper quasiparticle band.

Figure 2 shows the contour plot for the spectral intensity \( A(k, \omega) \) along the high-symmetry lines of the Brillouin zone. The quasiparticle band appears at the bottom (top) of the upper (lower) band for \( n = 1.00^+ \). The AF shadow bands with rather weak intensity appear along X-\( \Gamma \)-M’ (M’-M-X) in the upper (lower) band. Upon doping, the in-gap states at \( \omega - \mu \sim -t \) together with the upper quasiparticle band acquire the features of a renormalized quasiparticle band similar to that in the paramagnetic phase.

Upon doping the chemical potential moves higher in the upper quasiparticle band, and small Fermi surface pockets appear close to the X-points as also found in
ical potential. The shape of the strongest intensity corre-
sponds to Fermi surfaces. Upon doping the small Fermi
surface pockets appear first around the X-points. As
the doping increases these Fermi surface pockets deform
and become pieces of the paramagnetic-like Fermi sur-
face. The dashed line in Fig. 4 for $n = 1.12$ denotes the
Fermi surface of the non-interacting tight-binding disper-
sion in the paramagnetic phase. The form of the Fermi
surface deformation with doping agrees qualitatively with
the ARUPS measurement [11].

In order to elucidate the origin and the nature of the in-
gap state, we consider a simple variational wavefunction
[26]. The MF ground state is expressed by filling up the
states below the chemical potential,

$$|0\rangle = \prod_k \prod_m \prod_\sigma \theta(\mu_0 - E_{km})|\gamma_k^\dagger\rangle|\text{vac}\rangle,$$

where the MF-quasiparticle $\gamma$-operator is related to
the $c$-operator by $\gamma_k = \sum_{\sigma} \sqrt{v_{km}} |\gamma_k\rangle$ with $v_{km} =
\sqrt{(1 - m^2\xi_k/E_k^2)/2}$. The quasihole MF state in the lower
band is described by $|p\sigma-\rangle = \gamma_{p\sigma-}|0\rangle$, which couples
with multiple spin exchange states via the residual Hub-
bard interaction, $H_{\text{int}}$.

Consider the variational wavefunction defined by

$$|\Psi_{p\sigma-}\rangle = \sin\theta_p|p\sigma\rangle - \cos\theta_p|\phi_{p\sigma}\rangle,$$

where $|\phi_{p\sigma}\rangle$ contains multiple spin excitations and $\theta_p$ is a variational parameter. A basic component of the $|\phi_{p\sigma}\rangle$
is then given by applying $H_{\text{int}}$ on $|p\sigma-\rangle$, which generates
states with a particle-hole spin excitation. Among these
states, the state involving a particle-hole spin excitation
within the upper band makes the dominant contribution
which lowers the energy of the $|\Psi_{p\sigma-}\rangle$, i.e.,

$$|\phi_{p\sigma}\rangle = \frac{1}{\sqrt{A_p N}} \sum_{k,q} f(p, k; q)\gamma_{p+q\sigma+qk-q\sigma+\gamma_k^\dagger}|0\rangle,$$

where

$$f(p, k; q) = p_-(p + q, p)p_+(k - q, k) - |q \rightarrow q + Q|,$$

with the coherent factor $p_{\pm}(k, k') = v_{k+}v_{k'\pm} \pm v_{k-}v_{k'\mp}$. Here $A_p$ is the appropriate normalization factor.

Minimizing the total energy $E_p^{\text{tot}} = \langle\Psi_{p\sigma-}|H|\Psi_{p\sigma-}\rangle$ with respect to $\theta_p$, we obtain the renormalized quasihole energy, $E_{p\sigma-} = (E_p^{\text{tot}} - E_0)$, where $E_0 = \langle0|H|0\rangle$. For small doping two holes in the $|\phi_{p\sigma}\rangle$ have a momentum close to the X-points, i.e., $p + q \sim k - q \sim X$. Due to the momentum conservation the momentum of the particle is $k \sim p$. Since the kinetic energy of the $|\phi_{p\sigma}\rangle$ is the order of $E_{p\sigma-} - \mu_0$ and the average of the Coulomb interaction is negligible, the average of the total energy of the $|\phi_{p\sigma}\rangle$ is the order of $E_{p\sigma-} - \mu_0$, which is the order of $U$ smaller than that of the hole in the lower band, $|p\sigma-\rangle$. Therefore, the

The shape of the strongest intensity corre-

FIG. 3: The spectral intensity along $\Gamma(0, 0)$-$M(\pi, \pi)$ line. As
the doping increases, the in-gap states develop and become
dispersive. The in-gap states and the upper quasiparticle
band exhibit features of a renormalized quasiparticle band
similar to that in the paramagnetic phase.

FIG. 4: The contour plot of $A(k, 0)$ at the chemical poten-
tial corresponding to a Fermi-surface plot. Upon doping the
small Fermi surface pockets appear first around the X-points.
As the doping increases these pockets deform and become
pieces of the paramagnetic-like Fermi surface indicated by the
dashed line for $n = 1.12$.

the strong coupling calculations of Ref. [11]. These small
pockets provide new decay channels through the creation
of the particle-hole spin excitations in the upper quasi-
particle band. Then, a redistribution of the spectral
weight again takes place particularly in the lower band,
leading to a considerable reduction as shown in Figs. 4
and 5 which must be compensated by the appearance of
spectral weight elsewhere, i.e., in the in-gap state that
appears at $\omega - \mu \sim -t$. With further doping, the in-gap
states become more visible in wide regions of the BZ,
while the shadow bands become less visible except close
to the chemical potential. As a result, the in-gap states
together with the upper quasiparticle band exhibit clear
resemblance to a renormalized quasiparticle band in the
paramagnetic phase with the pseudogap due to strong
AF fluctuations (so-called hot spots) [21, 22, 23, 24, 25].
This is seen more clearly in Fig. 4 in which the in-gap
states develop and become dispersive with doping.

Figure 4 shows the contour plot of $A(k, 0)$ at the chem-
ical potential. The shape of the strongest intensity corre-
In Fig. 5, we compare the quasihole energies for $n = 1.12$ (a) evaluated by the variational wavefunction with (b) the results of the SCBA calculation in the quasiparticle $\gamma$-representation. The green (red) line in Fig. 5(a) represents the renormalized (MF) quasihole band. The dispersion of the renormalized quasihole band in Fig. 5(a) follows the curve $-E_{p_+}$. The variational evaluation of the quasihole energy agrees reasonably closely with the SCBA results except for region close to the $\Gamma$-point. Since the states near the $\Gamma$-point are far from $\mu_0$, the simple variational wavefunction would be poor. Note that a similar variational argument could be hold for hole dopings, where small hole pockets around the zone diagonals are involved instead (see Fig. 2).

Since the renormalization of the order parameter is neglected in this work, the AF phase survives up to a larger doping than the actual value ($n_c \sim 1.12$). However in reality, there exist well developed short-range order and strong AF fluctuations. As the ARPES experiment is insensitive against the difference between a short-range order and true long-range order, our treatment with an unrenormalized MF order parameter mimics the presence of short-range order. Nevertheless, the renormalization could be important for the smooth evolution of the Fermi surface near $n_c$ accompanied by the appearance of spectral weight around the zone diagonals [11, 12]. These features are reproduced by MF approaches with renormalization of the ordered moment [12]. A more sophisticated theoretical treatment is needed to describe this smooth evolution of the spectra as the AF order changes rapidly from long to short range.

In summary, we have studied systematically the evolution of the single-particle spectrum in the doped antiferromagnetic insulator. Starting from the MF antiferromagnetic insulator, we take into account multiple exchange of transverse spin excitations in the self energy. Away from half-filling we observe small Fermi surface pockets near the X-points and simultaneously the in-gap quasiparticle states, which eventually evolve into a renormalized quasiparticle band similar to that in the paramagnetic phase. We have proposed the simple variational wavefunction for the in-gap state, where the lower quasihole state admixes strongly with the upper quasihole state accompanied by a particle-hole excitation in the upper quasiparticle band. We have demonstrated that the weak-coupling treatment starting from the AF insulator gives a good description of the single-particle spectrum of the electron-doped cuprates.

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