Non-Fermi-liquid behavior for holes in doped two-dimensional antiferromagnets

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Spin and hole excitations are investigated in the doped two-dimensional (2D) antiferromagnets described by the *t-J* model based on the spin-wave approximation. The polarizability of spin excitations is found to be consistent with the marginal-Fermi-liquid hypothesis. As a consequence, the imaginary part of the self-energy for holes scattered by the spin excitations is demonstrated to give a linear dependence in temperature T (for $\omega < T$) and in frequency ω (for $\omega > T$).

It has been realized that the anomalous normal-state properties in the high-T_c cuprates are difficult to explain in the framework of the conventional Landau Fermi-liquid (FL) theory. There is a rising interest in two-dimensional (2D) models which possess low-energy noncanonical Fermi-liquid properties.

The most striking normal-state properties of the cuprate superconductors, which deviate from the conventional FL behavior, are that the resistivity is linear in T over a wide temperature range[1] and the inverse electron lifetime $\tau^{-1}(\mathbf{k},\omega)$ seems to be proportional to the frequency ω.[2] The phenomenological marginal-Fermi-liquid (MFL) theory proposed by Varma *et al.*[3] showed that quite a number of experimental results can be explained by use of a single hypothesis: the characteristic frequency and temperature dependence of polarizability for both charge and spin-density excitations. It has been shown[4] that MFL behavior can come about if the quasiparticles scatter from an assumed bosonic spectrum which is flat over a frequency scale from $T<\omega<\omega_c$ (ω_c is the cutoff frequency), but the origin of the bosonic spectrum is not yet clear. Aristov *et al.*[7] have observed a crossover from Fermi-liquid to Luttinger-liquid-like behavior in the 2D small-U Hubard model, and argued that it reproduced in the fermionic channel of the *t-J* model. However, because of the interaction between holes and spin excitations in the doped antiferromagnet, it is important to consider the behavior of holes (fermions) in the channel of the fermion-boson (spin excitations) interactions. In this paper, we show that, under adequate assumptions, the hole quasiparticles formed by the hole doping in 2D antiferromagnets behave as a noncanonical Fermi liquid when they are scattered by the spin excitations, and the polarizability arising from the damping of spin excitations into particle-hole pairs has the same form as the MFL hypothesis.

The physics of undoped high-T_c cuprates are well described by an isotropic, spin-$\frac{1}{2}$ Heisenberg model on a square lattice. Hole doping quickly destroys the long-range antiferromagnet (AF) order and eventually gives rise to the metallic state with a superconductive ground state at a small hole concentration. The essential aspects of the low-energy dynamics of a doped 2D antiferromagnet may be described by the so-called *t-J* model with the Hamiltonian given by

$$H=-t\sum_{\langle ij\rangle\sigma}(C_{i\sigma}^{+}C_{j\sigma}+\mathrm{H.c.})+J\sum_{\langle ij\rangle}\left[\mathbf{S}_i\cdot\mathbf{S}_j-\frac{n_in_j}{4}\right]. \tag{1}$$

Here $\langle ij\rangle$ indicates pairs of nearest neighbors, $n_i=\sum_\sigma C_{i\sigma}^{+}C_{i\sigma}$ and $C_{i\sigma}^{+}, C_{i\sigma}$ are creation and annihilation operators of electrons with the constraint of no double occupied sites, and $\mathbf{S}_i$ is the electronic spin operator at site i.

We consider a 2D square lattice with spin $\frac{1}{2}$. At finite temperatures or a small hole concentration, the system has no long-range order. Nevertheless, it has been shown[5] that the dynamical properties of the quasiparticles depend only on the short-range order, and come out practically the same with or without long-range order. So, to make the problem tractable, we divide the lattice into two sublattices (spin-up and spin-down), and apply the linear-spin-wave (LSW) approximation for the spin fluctuations, which gives reasonable results in comparison with the exact calculations on small clusters.[6,8–10]

We define the fermion operator f_i^+ which generates a hole at site i, and the boson operator b_i, such that $S_i^+=(1-f_i^+f_i)b_i$ on the spin-up sublattice and $S_i^-=(1-f_i^+f_i)b_i$ on the spin-down sublattice.[11] With these definitions and in the LSW approximation, the Hamiltonian (1) can be changed into

$$\begin{aligned}H=&-t\sum_{\langle ij\rangle}f_if_j^+(b_i^++b_j)+\mathrm{H.c.}\\&+\frac{1}{2}J\sum_{\langle ij\rangle}(1-f_i^+f_i)(1-f_j^+f_j)\\&\qquad\times[b_i^+b_i+b_j^+b_j+b_ib_j+b_i^+b_j^+-1]\,.\end{aligned} \tag{2}$$

The hopping part of the Hamiltonian preserves the constraint of no double occupancy because $f_i b_i = 0$. The factor $(1-f_i^+ f_i)(1-f_j^+ f_j)$ projects out the antiferromagnetic coupling when one or two sites of nearest-neighbor pairs are occupied by a hole. It introduces the disorder effect on the antiferromagnetic background and accounts for a loss of magnetic energy due to hole doping. The calculations[12] have shown that, for low concentrations of dopant holes, the softening of spin waves is mainly due to the strong coupling of spin waves to doped holes, the perturbations produced by solitary holes in the spin system is less important. We may replace $(1-f_i^+ f_i)(1-f_j^+ f_j)$ by 1.

The standard Fourier transformation and the Bogoliubov transformation for spin-wave variables gives

$$H=\sum_q \omega_q^0 \beta_q^+ \beta_q - \mu_f \sum_k f_k^+ f_k + \left[\frac{1}{N}\right]^{1/2} \sum_{kq} [f_{k-q}^+ f_k (g_{kq}\beta_q^+ + g_{k-q,-q}\beta_{-q}) + \text{H.c.}] \tag{3}$$

with

$$\omega_q^0 = J(1-\gamma_q^2)^{1/2}/2, \quad g_{kq} = t(\gamma_{k-q}u_q + \gamma_k v_q),$$

$$u_q = \left[\frac{1+(1-\gamma_q^2)^{1/2}}{2(1-\gamma_q^2)^{1/2}}\right]^{1/2},$$

$$v_q = -\text{sign}(\gamma_q)\left[\frac{1-(1-\gamma_q^2)^{1/2}}{2(1-\gamma_q^2)^{1/2}}\right]^{1/2}.$$

We have set $t = zt$, $J = zJ$, with z the number of nearest neighbors. Here, $\gamma_k = (\cos k_x + \cos k_y)/2$, μ_f is the chemical potential of holes, and N the number of lattice sites.

Introducing the Matsubara Green's functions for holes and spin waves, respectively,

$$G(\mathbf{k},\tau) = -\langle T_\tau f_k(\tau) f_k^+(0)\rangle , \tag{4}$$

$$D(\mathbf{k},\tau) = -\langle T_\tau \beta_k(\tau) \beta_k^+(0)\rangle . \tag{5}$$

Then, from the Hamiltonian (3) we can obtain the Dyson's equations for these Green's functions. After an analytical continuation to the upper half part of the complex plane, we can write the retarded Green's functions and self-energies for holes and spin excitations as[13]

$$G_R(\mathbf{k},\omega) = [\omega + \mu_f - \Sigma_R(\mathbf{k},\omega)]^{-1} , \tag{6}$$

$$D_R(\mathbf{q},\omega) = [\omega - \omega_q^0 - \Pi_R(\mathbf{q},\omega)]^{-1} , \tag{7}$$

$$\Sigma_R(\mathbf{k},\omega) = -\frac{1}{(2\pi)^3\pi}\int d^2p \int_{-\infty}^{\infty} d\omega_n \int_{-\infty}^{\infty} dx \left[\tanh\left[\frac{\omega_n}{2T}\right] + \coth\left[\frac{x}{2T}\right]\right] g_{k,k-p}^2 \frac{\text{Im}D_R(\mathbf{k}-\mathbf{p},x)\,\text{Im}G_R(\mathbf{p},\omega_n)}{x-\omega+\omega_n - i\delta} , \tag{8}$$

$$\Pi_R(\mathbf{q},\omega) = \frac{1}{(2\pi)^3\pi}\int d^2k \int_{-\infty}^{\infty} d\omega' \int_{-\infty}^{\infty} dx \left[\tanh\left[\frac{\omega'}{2T}\right] - \tanh\left[\frac{x}{2T}\right]\right] g_{k,q}^2 \frac{\text{Im}G_R(\mathbf{k},x)\,\text{Im}G_R(\mathbf{k}-\mathbf{q},\omega')}{x-\omega'-\omega-i\delta} , \tag{9}$$

where we have substituted the vertex functions (the sum of all diagrams which connect one spin excitation and two hole lines) by the bare vertex g_{kq}, because recently Sherman and Schreiber[14] have shown that the Migdal theorem[15] is also valid for the system considered above.

The motion of holes in a 2D quantum antiferromagnet has been investigated entensively.[11,16–18] The results for the dynamics of holes obtained so far may be summarized as (1) a single hole becomes mobile in the spin background and is accompanied by spin distortion around it; (2) the hole spectrum is strongly renormalized by the interaction with the spin excitations and that the holes can be described by a narrow quasiparticle band with a bandwidth of order J; (3) the quasiparticle energy has its minimum value at the points $(\pm\pi/2,\pm\pi/2)$ in the Brillouin zone. According to the above results, we will assume that hole quasiparticles form a weakly interacting Fermi gas. In the vicinity of four minima $(\pm\pi/2,\pm\pi/2)$, the quasiparticle energy ϵ_k can be expanded as[5,6]

$$\epsilon_k = \epsilon_{k_i} + \frac{1}{2m}k'^2 , \tag{10}$$

where $\mathbf{k}'$ is given by $\mathbf{k}=(\pm\pi/2,\pm\pi/2)+\mathbf{k}'$, with $|\mathbf{k}'|\ll 1$, and ϵ_{k_i} are the quasiparticle energies at four minima, m is the effective mass of hole quasiparticles $m \approx 3.8/t$, for $J/t = 0.3$.[5] As a starting point, the hole Green's function (6) may be approximated by the one-pole expression

$$G_R(\mathbf{k},\omega) \approx \frac{Z_k}{\omega - \epsilon_k + \mu_f + i\delta} . \tag{11}$$

The quasiparticle residue Z_k is determined from Eq. (8) with $D_R(\mathbf{k},\omega)$ replaced by $D_R^0(\mathbf{k},\omega)$ (the noninteracting Green's function for spin excitations), one finds,[14] $Z_k^2 \approx 2(J/t)^2/\pi$.

The Fermi surface of holes for finite hole concentrations is shown in Fig. 1, inside of which the number of states equals the number of holes, so the Fermi wave vector of holes is of the form $k_F^2 \approx \pi\delta$, with δ the hole concentration.

As for the spin excitations, we consider the wave vector $\mathbf{q}$ near $\Gamma(0,0)$ point, i.e., the case of long-wavelength excitations, such that $|\mathbf{q}| \ll 1$.

Because k' and q are all small, the interaction constant $g_{k_q}^2$ [see Eq. (12) for reference] can be approximated by

$$g_{kq}^2=\sum_{i=1}^{4} g_{k_i q}^2=\frac{t^2}{2\sqrt{2}}(qk'^2-2\sqrt{2}\mathbf{q}\cdot\mathbf{k}'+2q) . \qquad (12)$$

Inserting Eqs. (11) and (12) into Eq. (9), we obtain the imaginary part of self-energy for spin excitations

$$\mathrm{Im}\Pi_R(\mathbf{q},\omega)=\frac{Z_k^2 t^2 q}{16\sqrt{2}\pi}\int k'dk'\int d\theta(k'^2-2\sqrt{2}k'\cos\theta+2)\left[\tanh\left[\frac{\epsilon_k-\mu_f-\omega}{2T}\right]-\tanh\left[\frac{\epsilon_k-\mu_f}{2T}\right]\right]\delta(-\omega+\epsilon_k-\epsilon_{k-q}) . \qquad (13)$$

Performing the integration over k' in Eq. (13), one finds

$$\mathrm{Im}\Pi_R(\mathbf{q},\omega)=\frac{Z_k^2 t^2 m}{8\sqrt{2}\pi}\int_0^{\theta_m} d\theta\frac{K_m}{\cos^2\theta}\left[\frac{K_m^2}{\cos^2\theta}-2\sqrt{2}K_m+2\right]\left[\frac{1}{e^{(K_m^2/\cos^2\theta-k_F^2)/2mT}+1}-\frac{1}{e^{(K_m^2/\cos^2\theta-k_F^2-2m\omega)/2mT}+1}\right] , \qquad (14)$$

where $K_m=m(\omega+q^2/2m)/q<k_F\sim O(\delta^{1/2}),\theta_m$ is determined by $\cos\theta_m=m(\omega+q^2/2m)/k_F q$.

First, we consider the case $\omega/T<1$, then the imaginary part of self-energy of spin excitations is approximated by

$$\mathrm{Im}\Pi_R(\mathbf{q},\omega)=\frac{Z_k^2 t^2 m^2 K_m T}{4\sqrt{2}\pi}\int_0^{\theta_m} d\theta\left[\frac{K_m^2}{\cos^2\theta}-2\sqrt{2}K_m+2\right]\left[\frac{1}{(4mT-k_F^2)\cos^2\theta+K_m^2}-\frac{1}{(4mT-k_F^2-2m\omega)\cos^2\theta+K_m^2}\right] . \qquad (15)$$

The straightforward calculation gives

$$\mathrm{Im}\Pi_R(\mathbf{q},\omega)=-\frac{Z_k^2 t^2 m k_F}{16\sqrt{2}\pi}\frac{\omega}{T}(1-\sqrt{2}K_m)\sqrt{1-(K_m/k_F)^2} . \qquad (16)$$

Second, for the case $\omega/T>1$, the imaginary part of $\mathrm{Im}\Pi_R(\mathbf{q},\omega)$ in Eq. (14) can be represented in the form

$$\mathrm{Im}\Pi_R(\mathbf{q},\omega)=\frac{Z_k^2 t^2 m K_m}{8\sqrt{2}\pi}\int_0^{\theta_m} d\theta\frac{1}{\cos^2\theta}\left[\frac{K_m^2}{\cos^2\theta}-2\sqrt{2}K_m+2\right]\left[\frac{2mT\cos^2\theta}{(4mT-k_F^2)\cos^2\theta+K_m^2}-1+e^{(K_m^2/\cos^2\theta-k_F^2-2m\omega)/2mT}\right] . \qquad (17)$$

Performing the integration over θ, one finds,

$$\mathrm{Im}\Pi_R(\mathbf{q},\omega)=-\frac{Z_k^2 t^2 m k_F}{8\sqrt{2}\pi}(1-\sqrt{2}K_m)\times\left[1-\frac{k_F^2-K_m^2}{8mT}-e^{-\omega/T}\right]\times\sqrt{1-(K_m/k_F)^2} . \qquad (18)$$

For both the cases, neglecting terms of $O(k_F^3)\sim O(\delta^{3/2})$, we obtain

$$\mathrm{Im}\Pi_R(q,\omega<T)=-\frac{Z_k^2 t^2 m k_F}{16\sqrt{2}\pi}\left[\frac{\omega}{T}\right] ,$$
$$\mathrm{Im}\Pi_R(\mathbf{q},\omega>T)=-\frac{Z_k^2 t^2 m k_F}{8\sqrt{2}\pi} . \qquad (19)$$

The polarizability (19) has the same form as the MFL hypothesis.[3,4] Yet, unlike the second-order perturbation calculations in the electron-electron interaction, what comes into the calculation of the self-energy of holes here is the imaginary part of the Green's function for spin excitations, i.e., the spectrum for spin excitations, as can be

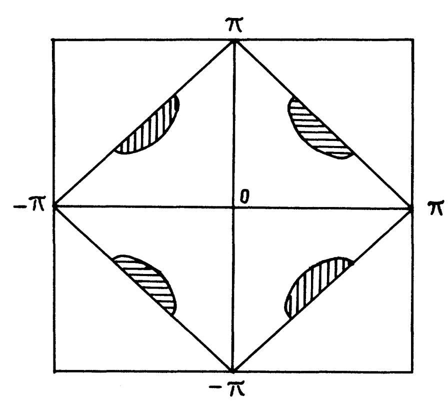

FIG. 1. A schematic plot for the Fermi surface of holes at low concentrations in the reduced Brillouin zone.

seen from Eq. (8). So, we will first evaluate the real part of the self-energy for spin excitations in the following.

Performing the similar calculations, we can find the real part of the self-energy $\Pi_R(\mathbf{q},\omega)$ in the limits of our interest,

$$\mathrm{Re}\Pi_R(\mathbf{q},\omega)=-\frac{Z_k^2t^2mq}{8\sqrt{2}\pi}\left[1+\frac{k_F^2}{2}\right]+\frac{Z_k^2t^2m^2}{8\pi}\omega\ . \qquad (20)$$

Thus the spectrums for spin excitations which is involved in the calculations of hole self-energies are given by

$$\begin{aligned}\mathrm{Im}D_R(\mathbf{q},\omega<T)&\approx-\frac{Ck_F\omega}{\{(1-2\sqrt{2}mc)\omega-[\sqrt{2}J-C(2+k_F^2)]q\}^2T}\ ,\\ \mathrm{Im}D_R(\mathbf{q},\omega>T)&\approx-\frac{2Ck_F}{\{(1-2\sqrt{2}mc)\omega-[\sqrt{2}J-C(2+k_F^2)]q\}^2}\end{aligned} \qquad (21)$$

with $C=Z_k^2t^2m/16\sqrt{2}\pi\approx\sqrt{2}mJ^2/\pi^2\approx0.16J$.

The imaginary part of hole self-energies $\mathrm{Im}\Sigma_R$ which arises from the scattering from spin excitation spectrum given in Eq. (21), may be evaluated from Eq. (8),

$$\mathrm{Im}\Sigma_R(k,\omega)=-\frac{Ck_FZ_kt^2}{8\sqrt{2}\pi^2}\int dp'\frac{p'(k'^2+p'^2)}{k'-p'}\left\{\int_{-T}^{T}dx\frac{x}{T}M(x)+\int_{T}^{\infty}dx\,M(x)+\int_{-\infty}^{-T}dx\,M(x)\right\}, \qquad (22)$$

where

$$M(x)=\frac{\{\tanh[(\omega-x)/2T]+\coth(x/2T)\}\delta(\omega-x-\epsilon_p+\mu_f)}{[F(x,k',p')]^2}$$

and

$$F(x,k',p')=(1-2\sqrt{2}mc)x-\sqrt{2}[1-mJ(2+k_F^2)/\pi^2]J(k'-p')\ .$$

For hole states near the Fermi surface, which give the essential contributions to the transport properties, we can expand $\epsilon_p-\mu_f\approx(p'-k_F)k_F/m$. Since for low hole concentrations, the velocity of spin excitations is larger than that of holes near the Fermi surface, i.e., $mJ/k_F\approx1/k_F>1$, we can approximate

$$F(x,k',p')\approx-\sqrt{2}[1-mJ(2+k_F^2)/\pi^2]J(k'-p')\ .$$

Then, from Eq. (22), we find,

$$\begin{aligned}\mathrm{Im}\Sigma_R(\mathbf{k},\omega>T)&\approx-\frac{mk_FJt}{2\sqrt{2}\pi^{5/2}[\pi^2-mJ(2+k_F^2)]^2}\omega\ ,\\ \mathrm{Im}\Sigma_R(\mathbf{k},\omega<T)&\\ &\approx-\frac{mk_FJt}{2\sqrt{2}\pi^{5/2}[\pi^2-mJ(2+k_F^2)]^2}(1+\ln2)T\ .\end{aligned} \qquad (23)$$

Thus our calculations provides an explanation for the linear temperature dependence of the resistivity, and for the linear frequency variation of the inverse hole lifetime, which is an indication of noncanonical Fermi-liquid behavior for holes.

It should be noted that the quasiparticle peak of holes occurs at the low frequencies ($\omega\leq J$), above this quasiparticle band, there is the incoherent part of hole spectrum ($\omega>J$), which was shown to be important for the softening of spin waves.[5,16,19] In the evaluations of polarizability, we just consider the coherent part of hole spectrum as shown in Eq. (11), so one would wonder if the results obtained in Eq. (19) will be changed when the incoherent part of the hole spectrum is taken into account. However, to our knowledge, there is no explicit expression presented for the incoherent spectrum of holes. In order to estimate the effect, we adopt the approximate form given by Khaliullin and Horsch,[19]

$$\mathrm{Im}G_R^{\mathrm{inc}}(\mathbf{k},\omega)=-\frac{1}{2\Gamma}\theta(|\omega|-J)\theta(2\Gamma-\omega) \qquad (24)$$

with $\Gamma\sim zt$. This leads to the contribution to polarizability from the transitions within the incoherent spectrum,

$$\mathrm{Im}\Pi_R^{\mathrm{II}}(\mathbf{k},\omega)=-\frac{qk_F^2t^2T}{64\sqrt{2}\pi^2\Gamma^2}\times\left[2\ln\left[\frac{\exp(-J/T)+1}{\exp[-(J+\omega)/T]+1}\right]+\ln\left[\frac{\exp(-2\Gamma/T)+1}{\exp[-(2\Gamma-\omega)/T]+1}\right]\right]. \qquad (25)$$

Another contribution is provided by the transitions between the incoherent spectrum and quasiparticle band, its leading term is given by

$$\mathrm{Im}\Pi_R^{\mathrm{CI}}(\mathbf{q},\omega)\approx-\frac{Z_kt^2mq}{8\sqrt{2}\pi}\left[\frac{\omega-J}{\Gamma}\right]\quad\text{for }\omega-J>T\ . \qquad (26)$$

It is obvious $\Gamma/T\gg1$. For the typical value of superchange coupling constant in high-T_c cuprates $J\approx1.3\times10^3$ K, we have $J/T>1$ in the range of our interest. So, provided we limit the range of frequencies of spin excitations to $\omega < \omega_C = t + J \approx 5.6 \times 10^3$ K (it introduces the cutoff frequency ω_C for the spectrum of spin excitations considered here), we can expect the incoherent part of hole spectrum will not change our results obtained above.

The essential difference between our model and the standard calculations of the electron-boson interaction is the four pocketlike Fermi surfaces of holes situated at the points $(\pm\pi/2, \pm\pi/2)$ in the Brillouin zone. It is derived from the self-consistent perturbation calculations of the motion of one-hole in an antiferromagnet background at zero temperature[11,16] and also at finite temperatures.[6] In other words, the effect of strong correlations is believed to be included when this special Fermi surface of holes is taken in the calculations. As the first step, we can treat the hole quasiparticles as a weakly interacting Fermi gas. On the other hand, with a finite concentration of holes, the spectrum of spin excitations will change due to the interaction between hole quasiparticles and spin excitations. It turns out that the polarizability of spin excitations has the same form as the marginal-Fermi-liquid hypothesis, and leads to the linear dependence in ω (for $\omega > T$) or T (for $T > \omega$).

In summary, we have shown that the interaction between holes and spin excitations associated with the generation of particle-hole pairs may lead to the noncanonical Fermi-liquid behavior for holes in doped two-dimensional antiferromagnets. The special pocketlike Fermi surface of holes, which contains the effect of strong correlations, may be responsible for the behavior of holes.

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