Spectral function of small spin polaron in two-dimensional spherically symmetric antiferromagnetic state

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The spectral density $A_p(k,\omega)$ of a small spin polaron in the CuO_2 plane is calculated in the self-consistent Born approximation within the framework of the three-band model. It is shown that the spin polaron is a good quasiparticle excitation for this model. $A_p(k,\omega)$ demonstrates small damping in contrast to $A_h(k,\omega)$ for a bare hole, and the lowest boundary $\omega_{p,\min}$ of $A_p(k,\omega)$ lies much lower than $\omega_{h,\min}$ for $A_h(k,\omega)$. The quasiparticle peak dispersion reproduces the flat region near the band bottom that is characteristic of the bare polaron spectrum Ω_k. The spherically symmetric approach is used for description of spin excitations. It makes it possible to consider the quantum antiferromagnetic background without the spontaneous symmetry breaking and the unit cell doubling. [S0163-1829(97)04404-4]

Up to date much theoretical work has been devoted to the problem of a hole motion in two-dimensional (2D) $s=1/2$ quantum antiferromagnetic (AFM).[1] The important question is whether a hole injected in the undoped ground state behaves like a quasiparticle (QP). This problem is mainly investigated within the framework of the t-J model[2–7] and there are rather few works devoted to the three-band Hubbard model or the Emery model[8,9] that is more realistic for CuO_2 planes in high-T_c superconductors (HTSC). For the t-J model it was shown that the spectral density function $A_h(k,\omega)$ of a doped hole revealed a QP peak of intensity $Z_k \approx J/t$ and a broad incoherent part that has a width of about $6t$–$7t$. The QP band bottom corresponds to the momenta $\mathbf{k}_1=(\pm\pi/2,\pm\pi/2)$. Similar results were obtained for the Emery model.[11–13] The presence of a great incoherent part and small intensity of QP peak indicate that bare holes are rather poor elementary excitations even for $\mathbf{k}$ close to $\mathbf{k}_1$.

The elementary excitations in the CuO_2 plane are known to be described within the framework of the spin polaron concept. In the Emery model the mean-field spectrum Ω_k of a bare small spin polaron demonstrates a flat band region close to the magnetic Brillouin zone boundary.[14] This region corresponds to the bottom of the band and it arises due to the hole moving in the antiferromagnetic background.

In the present paper we study the spectral density function $A_p(k,\omega)$ of a small spin polaron in the Emery model treating the coupling to spin-wave excitations within the self-consistent Born approximation (SCBA) for the corresponding two-time retarded Green's function $G(k,\omega)$. We show that (i) for the flat band region the QP peak of the spectral density function $A_p(k,\omega)$ is close to the bottom of the bare polaron Ω_k band and reproduces this flat region; (ii) the intensity of this peak is much higher and the damping much lower compared to the corresponding peak of $A_h(k,\omega)$ for a bare hole; (iii) the lowest boundary $\omega_{p,\min}$ of $A_p(k,\omega)$ lies much lower than $\omega_{h,\min}$ for $A_h(k,\omega)$. The distinctive feature of our investigation consists in considering the AFM copper spin subsystem in a spherically symmetric approach.[15,16] Such an approach is the most appropriate for considering the quantum two-dimensional (2D) AFM at any finite temperature. As a result the scattering of a spin polaron by spin excitations in the singlet spin background leads to the spectral function periodicity relative to the full Brillouin zone. Note that the conventional two-sublattice spin approach leads to periodicity relative to the magnetic (reduced) Brillouin zone.[2–7,12]

Following Refs. 8, 14, and 9 we adopt the Hamiltonian that corresponds to one-hole problem in the CuO_2 plane in HTSC:

$$\hat{H}=\tau\sum_{\mathbf{r},\mathbf{a}_1,\mathbf{a}_2,\sigma,\sigma'} c^{\dagger}_{\mathbf{r}+\mathbf{a}_1,\sigma}c_{\mathbf{r}+\mathbf{a}_2,\sigma'}\left(\frac{1}{2}\delta_{\sigma\sigma'}+2\mathbf{s}_{\sigma\sigma'}\mathbf{S}_{\mathbf{r}}\right)+\frac{J}{2}\sum_{\mathbf{r},\mathbf{g}}\mathbf{S}_{\mathbf{r}}\mathbf{S}_{\mathbf{r}+\mathbf{g}}, \tag{1}$$

$\mathbf{a}_1,\mathbf{a}_2=\pm\frac{1}{2}\mathbf{g}_x,\pm\frac{1}{2}\mathbf{g}_y,\mathbf{g}=\pm\mathbf{g}_x\pm\mathbf{g}_y$.

Here and below $\mathbf{g}_{x,y}$ are basic vectors of a copper square lattice ($|\mathbf{g}|\equiv 1$), $\mathbf{r}+\mathbf{a}$ are four vectors of O sites nearest to the Cu site $\mathbf{r}$, the operator $c^{\dagger}_{\sigma}$ creates a hole with the spin index $\sigma=\pm 1$ at the O site, $\mathbf{s}_{\sigma\sigma'}=\frac{1}{2}\boldsymbol{\sigma}_{\sigma\sigma'}$, operator $\mathbf{S}$ represents the localized spin on the copper site.

It is well known that the most prominent feature of the Hamiltonian (1) is that the low-energy physics of hole excitations is described by the Bloch sums $\mathcal{B}^{\dagger}_{k,\sigma}$ based on one site

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small polaron operators $\mathcal{B}^{\dagger}_{r\sigma}$ (the analogous of the so-called Zhang-Rice singlet in CuO_4 plaquette)[10,14]

$$\mathcal{B}^{\dagger}_{k,\sigma}=\frac{1}{\sqrt{NK_k}}\sum_{\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}}\mathcal{B}^{\dagger}_{r,\sigma}, \tag{2}$$

$$\mathcal{B}^{\dagger}_{r,\sigma}=\frac{1}{2}\sum_{\mathbf{a}} (c^{\dagger}_{r+a,\sigma}Z^{\overline{\sigma\sigma}}_{r}-c^{+}_{r+a,\bar{\sigma}}Z^{\sigma\bar{\sigma}}_{r}), \tag{3}$$

$$K_k=\left\langle \frac{1}{N}\sum_{\mathbf{r},\mathbf{r}'} e^{-i\mathbf{k}(\mathbf{r}-\mathbf{r}')}\{\mathcal{B}_{r,\sigma},\mathcal{B}^{\dagger}_{r',\sigma}\}\right\rangle=1+(C_g+1/4)\gamma_k .$$

Here $\{,\}$,$[,]$ stand for an anticommutator and commutator, respectively; $\bar{\sigma}=-\sigma$; $Z^{\sigma_1\sigma_2}_r$ are the Hubbard projection operators for Cu sites states; $\gamma_k=\frac{1}{4}\Sigma_g \exp(i\mathbf{k}\cdot\mathbf{g})$; $C_r=\langle \mathbf{S}_0\cdot\mathbf{S}_r\rangle$. Let us recall that in the spherically symmetric approach adopted here $\langle S^{\alpha}_i S^{\beta}_j\rangle=\delta_{\alpha\beta}\langle S^{\alpha}_i S^{\alpha}_j\rangle=\frac{1}{3}\langle \mathbf{S}_i\cdot\mathbf{S}_j\rangle$. Note that $\mathcal{B}^{+}_{k,\sigma}|L\rangle$ corresponds to the CuO_2 plane state with the total spin equal to $\frac{1}{2}$ if $|L\rangle$ is the singlet state. We treat $\mathcal{B}^{\dagger}_{k,\sigma}$ as a candidate for the elementary excitations operator and calculate the corresponding two-time retarded Green's function $G(k,\omega)$ and spectral density $A_p(k,\omega)=-(1/\pi)\mathrm{Im}G(k,\omega+i0^+)$,

$$G(k,\omega)=\langle \mathcal{B}_{k,\sigma}|\mathcal{B}^{\dagger}_{k,\sigma}\rangle_{\omega}$$

$$\equiv-\iota\int_{t'}^{\infty}dt e^{\iota\omega(t-t')}\langle\{\mathcal{B}_{k,\sigma}(t),\mathcal{B}^{\dagger}_{k,\sigma}(t')\}\rangle. \tag{4}$$

The Dyson's equation for $G(k,\omega)$ has the form

$$G^{-1}(k,\omega)=G_0^{-1}-\Sigma(k,\omega),\quad \Sigma(k,\omega)=\langle \mathcal{R}_{k,\sigma}|\mathcal{R}^{\dagger}_{k,\sigma}\rangle^{(\mathrm{irr})}, \tag{5}$$

where

$$G_0=(\omega-\Omega_k)^{-1},$$

$$\mathcal{R}_{k,\sigma}=[\mathcal{B}_{k,\sigma},H]=\frac{1}{\sqrt{NK_k}}\sum_{\mathbf{r}} e^{-i\mathbf{k}\cdot\mathbf{r}}\mathcal{R}_{r,\sigma}, \tag{6}$$

$$\mathcal{R}_{r,\sigma}=-4\tau\mathcal{B}_{r,\sigma}+\mathcal{R}^{\tau}_{r,\sigma}+\mathcal{R}^{J}_{r,\sigma}, \tag{7}$$

$$\mathcal{R}^{\tau}_{r,\sigma}=-\frac{\tau}{2}\sigma\Bigg(\sum_{\mathbf{g},\mathbf{a},\sigma_1}\sigma_1 Z^{\overline{\sigma\sigma_1}}_{r}c_{r+g+a,\bar{\sigma}_1}-\sum_{\mathbf{g},\mathbf{a},\sigma_1,\sigma_2}\sigma_2 Z^{\bar{\sigma}\sigma_1}_{r}Z^{\sigma_1\sigma_2}_{r+g}c_{r+g+a,\bar{\sigma}_2}\Bigg), \tag{8}$$

$$\mathcal{R}^{J}_{r,\sigma}=\frac{J}{4}\sigma\Bigg(\sum_{\mathbf{g},\mathbf{a},\sigma_1,\sigma_2}\sigma_1(Z^{\bar{\sigma}\sigma_2}_{r}Z^{\sigma_2\bar{\sigma}_1}_{r+g}-Z^{\bar{\sigma}\sigma_2}_{r+g}Z^{\sigma_2\bar{\sigma}_1}_{r})c_{r+a,\sigma_1}\Bigg)$$

$$\Omega_k=\langle\{\mathcal{R}_{k,\sigma},\mathcal{B}^{\dagger}_{k,\sigma}\}\rangle=(\tau Q_{\tau}+JQ_J)/K_k, \tag{9}$$

$$Q_{\tau}(k)=-\frac{7}{2}-8\left(\frac{1}{4}+C_g\right)\gamma_k+\left(\frac{1}{8}-C_g+\frac{1}{2}C_{2g}\right)\gamma_{2k}+2\left(\frac{1}{8}-C_g+\frac{1}{2}C_d\right)\gamma_{dk},$$

$$Q_J(k)=C_g(\gamma_k-4),$$

$$\langle\mathcal{R}|\mathcal{R}\rangle^{(\mathrm{irr})}=\langle\mathcal{R}_{k,\sigma}|\mathcal{R}^{\dagger}_{k,\sigma}\rangle-\langle\mathcal{R}_{k,\sigma}|\mathcal{B}^{\dagger}_{k,\sigma}\rangle\times\frac{1}{\langle\mathcal{B}_{k,\sigma}|\mathcal{B}^{\dagger}_{k,\sigma}\rangle}\langle\mathcal{B}_{k,\sigma}|\mathcal{R}^{\dagger}_{k,\sigma}\rangle. \tag{10}$$

Here and below $\mathbf{d}=\mathbf{g}_x+\mathbf{g}_y$, $\gamma_{dk}=\cos(k_x g)\cos(k_y g)$.

We see from Eqs. (5) and (10), that the self-energy $\Sigma(k,\omega)$ accounting for interaction effects is expressed through the higher-order Green's functions. One should notice, first, that the terms linear in $\mathcal{B}_{k,\sigma}$ do not contribute to the irreducible Green's function (10). Second, the lowest-order self-energy contribution is provided by the first term in the right-hand side of the expression (10), while the second term leads to higher-order corrections. Following Ref. 7 we evaluate (10) with a proper decoupling procedure for two time correlation function $\langle\mathcal{R}_{k,\sigma}(t)\mathcal{R}^{\dagger}_{k,\sigma}(t')\rangle$. This procedure is equivalent to the self-consistent Born approximation (SCBA) in a usual diagrammatic technique.[7] In our case this means that the two time correlation function is decoupled into the spin-spin correlation function and the polaron-polaron correlation function. The adopted decoupling procedure preserves the main character of polaron site operator (3)—four hole site operators surround the copper spin operator and it schematically has the form

$$\left\langle Z_{r_1}(t)\left(\sum_{a_1}c_{r_2+a_1}(t)Z_{r_2}(t)\right)\left(\sum_{a_2}Z_{r_3}(t')c^{\dagger}_{r_3+a_2}(t')\right)Z_{r_4}(t')\right\rangle\simeq\left\langle\left(\sum_{a_1}c_{r_2+a_1}(t)Z_{r_2}(t)\right)\left(\sum_{a_2}Z_{r_3}(t')c^{\dagger}_{r_3+a_2}(t')\right)\right\rangle\times\langle Z_{r_1}(t)Z_{r_4}(t')\rangle. \tag{11}$$

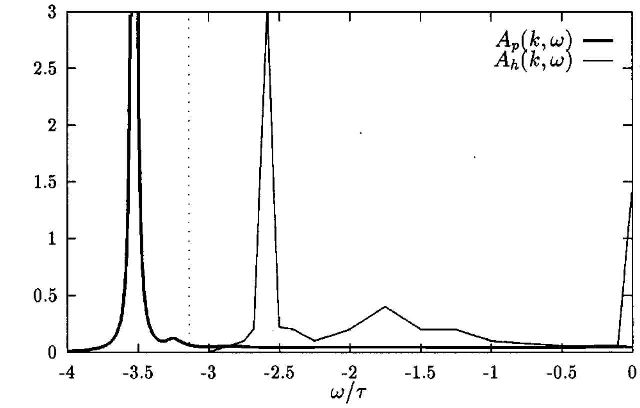

FIG. 1. Spin polaron spectral density $A_p(k_1,\omega)$, $k_1=(\pi/2,\pi/2)$, $J=0.7\tau$ (thick solid line) and $A_h(k_1,\omega)$ (thin solid line) schematically represents the spectral density for the bare hole from Ref. 12. The position of the spectral density function $A_0(k_1,\omega)$ peak for the bare (zero order) spin polaron Green's function $G_0(k,\omega)$ is represented by the vertical dotted line.

Let us mention that we also tested the more complex decoupling procedure, and it did not qualitively alter the results given by approximation (11). On the next step we project polaron operators in Eq. (11) onto $\mathcal{B}_{k\sigma}$:

$$c_i(t)Z_j(t)\simeq\xi\mathcal{B}_{k\sigma}(t),\quad \xi=\langle\{c_i(t)Z_j(t),\mathcal{B}^{\dagger}_{k,\sigma}\}\rangle. \quad (12)$$

The resulting correlation functions may be expressed through $G(k,\omega)$ and the spin excitation Green's function[15,16]

$$D(q,\omega)=\frac{1}{N}\sum_{\mathbf{r},\mathbf{r}'} e^{i\mathbf{q}(\mathbf{r}-\mathbf{r}')}\langle S^z_r|S^z_{r'}\rangle=-\frac{8JC_g}{3}\frac{1-\gamma_q}{\omega^2-\omega_q^2},$$

$$\omega_q^2=-32J\alpha_1C_g(1-\gamma_q)(2\Delta+1+\gamma_q); \quad (13)$$

here we neglect the influence of doped holes on spin dynamics and take the spin spectrum parameters calculated in Ref. 15 (the vertex correction $\alpha_1=1.7$, the spin excitations condensation part $m^2=0.0225$).

Finally, we come to the well-known integral equation for the Green's function that always arises within the framework of SCBA

$$G(k,\omega)=\frac{1}{\omega-\Omega_k-\Sigma(k,\omega)}, \quad (14)$$

where

$$\Sigma(k,\omega)=N^{-1}\sum_q M^2(k,q)[(1+\nu_q)G(k-q,\omega-\omega_q)$$

$$+\nu_qG(k-q,\omega+\omega_q)]. \quad (15)$$

$\nu_q=1/[\exp(\beta\omega_q)-1]$ is the Bose function and β is an inverse temperature.

$$M^2(k,q)=\frac{K_{k-q}}{K_k}\Gamma^2(k,q)\frac{(-4C_g)(1-\gamma_q)}{\omega_q}, \quad (16)$$

$$\Gamma(k,q)=\tau\Gamma_\tau(k,q)+\frac{J}{2}\Gamma_J(k,q),$$

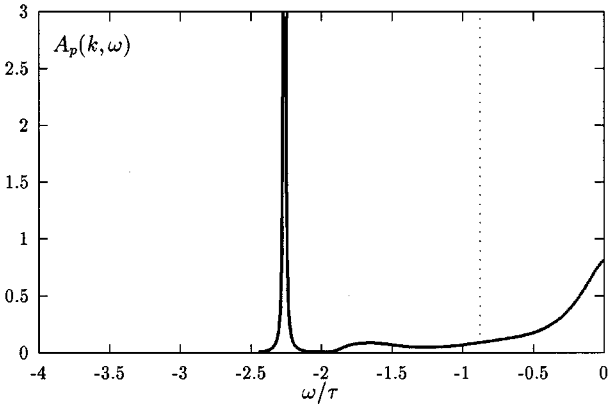

FIG. 2. Spin polaron spectral density $A_p(k_2,\omega)k_2=(0,0),J=0.7\tau$.

$$\Gamma_\tau(k,q)=4\gamma_{k-q}[(1+\gamma_{k-q})/2K_{k-q}-1],$$

$$\Gamma_J(k,q)=4\gamma_q\left[\left(\frac{3}{4}-C_g\right)\frac{4\gamma_{k-q}}{3K_{k-q}}-1\right].$$

$\Gamma(k,q)$ corresponds to the bare vertex for the coupling between a spin polaron and a spin wave. It is known[17] that this vertex is substantially renormalized for q close to the AFM vector $q_0=(\pi,\pi)$. This renormalization is due to the strong interaction of a polaron with the condensation part of spin excitations that must be taken into account from the very beginning. As a result, the renormalized vertex $\widetilde{\Gamma}(k,q)$ must be proportional to[17] $[(q-q_0)^2+L_s^{-2}]^{1/2}$, L_s being the spin-spin correlation length, $L_s\to\infty$ in our case of a long-range order state of the spin subsystem. Below this renormalization is taken into account empirically by the substitution

$$\Gamma(k,q)\to\widetilde{\Gamma}(k,q)=\Gamma(k,q)\sqrt{(1+\gamma_q)}. \quad (17)$$

The introduced vertex correction is proportional to $|\mathbf{q}-\mathbf{q}_0|$ for $\mathbf{q}$ close to $\mathbf{q}_0$. We have used also the following two functions for the vertex correction $\sqrt{1+\gamma_q^3}$ and $\sqrt{1+\gamma_q^5}$ and have obtained results similar to those presented below. Let us mention that the bare vertex leads the dramatic decrease of the QP bandwidth.

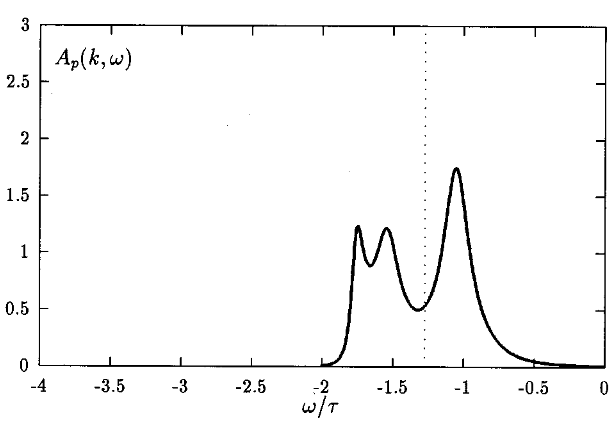

FIG. 3. Spin polaron spectral density $A_p(k_3,\omega)$ in $k_3=(\pi,\pi),J=0.7\tau$.

We calculate the spectral density $A(k,\omega)$ at $T=0$ by solving the self-consistent equation (14) on a 32×32 site lattice. A finite damping constant $\delta=0.01\tau$ is introduced, $\omega\to\omega+\iota\delta$. Instead of the usual iteration approach for numerical evaluation of Eq. (14) we use an alternative method based on the continued fraction expansion of $G(k,\omega)$.[18] The details of this procedure will be presented elsewhere. In Fig. 1 we show the spectral density $A_p(k,\omega)$ for the value of $\mathbf{k}_1=(\pi/2,\pi/2)$, which reproduce the low-energy excitation. In Figs. 2 and 3 $A_p(k,\omega)$ is given for $\mathbf{k}_{2,3}=(\pi,\pi),(0,0)$, which correspond to the top of the band. In these calculations the characteristic value of energetic parameter $J=0.7\tau$ is taken. To compare our results with the results for the bare hole $A_h(k,\omega)$ (Ref. 12) is also given for $\mathbf{k}_1=(\pi/2,\pi/2), J=0.7\tau$ in Fig. 1. The position of the spectral density function $A_0(k,\omega)$ peak for the bare (zero order) spin polaron Green's function $G_0(k,\omega)$ is also represented in the figures by the vertical dotted line.

As mentioned above, due to the AFM character of spin correlation functions, the Ω_k demonstrates a ''flat dispersion region'' close to the line $\gamma_k<0,|\gamma_k|\ll 1$.[14] In particular, the momentum k_1 is related to this flat region. As seen from Fig. 1, the spectral density function of this momentum has a sharp QP peak. Our calculation shows that $A_p(k,\omega)$ for k determined by the equation $\gamma_k=0$ are very close to the function given in Fig. 1. If we would consider ω_p, corresponding to the maximum of the peaks (analogous to the peak in the Fig. 1) as the QP energy, then we can conclude that QP energies also reproduce the flat region. This region also describes the bottom of the QP band. It may be seen from Fig. 1 that $A_p(k_1,\omega)$ demonstrates much sharper QP peaks relative to the results for a bare hole $A_h(k,\omega)$ in the *t-J* and Emery models.[4,12] For example, the pole strength $Z_p(k)$ [$Z_p(k)$ is the area under the peak] for the QP peak of Fig. 1 equals to $Z_p(k)=0.82$. The corresponding value for A_h given by Ref. 12 is much smaller, $Z_h(k)=0.25$.

As may be seen from Figs. 2 and 3, $A_p(k,\omega)$ for $k_2=(0,0)$ also demonstrate the QP peak with the pole strength $Z_p(k_2)=0.35$ in contrast to $k_3=(\pi,\pi)$ where no QP peak is observed. With the decrease of J value the lowest on ω peaks are preserved. The QP bandwidth determined by these peaks and the analogous peak for $k_1=(\pi/2,\pi/2)$ is of the order of J.

It is clear that for small J/τ the concept of a small spin polaron fails, and it is important to estimate the validity limits of this concept. Our calculations demonstrate that the intensity of QP peaks and the structure $A_p(k,\omega)$ do not change dramatically for k_1, corresponding to the band bottom, up to $J/\tau=0.1$. For example, $Z_p(\pi/2,\pi/2)\approx Z_p(\pi,0)\approx 0.50$ at $J/\tau=0.1$. So the J/τ lowest boundary value of the small spin polaron concept validity is lower than $J/\tau=0.1$.

Figure 1, $J=0.7\tau$, explicitly demonstrates the one-peak structure $A_p(k_1,\omega)$ in contrast to $A_h(k_1,\omega)$. It is also important that the bottom of our QP spectrum (value of ω_p corresponding to the center of the peak) $\omega_{p,\min}=-3.52\tau$ is substantially lower than $\omega_{\min,h}=-2.6\tau$ from Ref. 12 (note that our unit of energy is twice that of Ref. 12, $\tau=2t$). This result is a consequence of the fact that elementary excitation—spin polaron of small radii $\mathcal{B}_{k,\sigma}$—from the beginning takes into account the strong local hole-spin coupling.

To summarize, we have shown that spin polarons of small radius are good quasiparticles for realistic values of parameters in the Emery model. This means, in particular, that the problem of superconducting hole pairing must be treated as pairing of these quasiparticles rather then pairing of bare holes.

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