PECULIARITIES OF THE SPECTRUM OF STRONGLY CORRELATED ELECTRONS

A. SHERMAN
Institute of Physics, University of Tartu, Riia 142, 51014 Tartu, Estonia

AND

M. SCHREIBER
Institut für Physik, Technische Universität, D-09107 Chemnitz, Federal Republic of Germany and
School of Engineering and Science, International University Bremen, Campus Ring 1, D-28759 Bremen, Federal Republic of Germany

Abstract. Hole and spin Green’s functions of the two-dimensional $t$-$J$ model of the CuO$_2$ planes are calculated in an approximation which retains the rotation symmetry in the paramagnetic state and has no presumed magnetic ordering. In this approximation Green’s functions are represented by continued fractions which are interrupted by decouplings with a vertex correction determined from the constraint of zero site magnetization in the paramagnetic state. Obtained results are shown to be in good agreement with Monte Carlo and exact diagonalization data. The calculated spectra demonstrate a pseudogap and a band splitting which are similar to those observed in Bi-based cuprate perovskites.

For the description of strongly correlated electrons in CuO$_2$ planes of perovskite high-$T_c$ superconductors the two-dimensional $t$-$J$ model is widely used (for a review see Ref. [1]). One of the most fruitful analytical methods for this model uses the spin-wave description of magnetic excitations. Some spectral peculiarities obtained in this approach are similar to those revealed from the photoemission, spin-lattice relaxation and neutron scattering experiments (see, e.g., Ref. [2]). However, this approximation has two serious shortcomings: (i) deviations from the Néel state are presumed
to be small and (ii) the approximation violates the rotation symmetry of the paramagnetic state.

In this paper we try to overcome these difficulties by using the description in terms of spin and hole operators and the continued fraction representations for Green’s functions. Self-energies are calculated by decouplings corrected with the use of the constraint of zero site magnetization in the paramagnetic state. The Hamiltonian of the $t$-$J$ model reads

$$H = \sum_{nm} t_{nm} a^\dagger_n \sigma_m a_{m\sigma} + \frac{1}{2} \sum_{nm} J_{nm} \left( s^z_n s^z_m + s^+_n s^-_m \right) + \mu \sum_n X_n,$$

where $a_{n\sigma} = |n\sigma\rangle \langle n0|$ is the hole destruction operator, $n$ and $m$ label sites of the square lattice, $\sigma = \pm 1$ is the spin, $|n\sigma\rangle$ and $|n0\rangle$ are site states corresponding to the absence and presence of a hole on the site. In these notations the spin-$\frac{1}{2}$ operators are written as $s^z_n = \frac{1}{2} \sum_\sigma |n\sigma\rangle \langle n\sigma| s^z$ and $s^\sigma_n = |n\sigma\rangle \langle n,-\sigma|$. The hopping and exchange constants $t_{nm}$ and $J_{nm}$ are expected to be nonzero only for nearest neighbor sites for which they take the values $t$ and $J$. $\mu$ is the chemical potential and $X_n = |n0\rangle \langle n0|$.

The hole and spin Green’s functions are determined as follows:

$$G(k\omega) = -i\theta(\omega) \langle \{ a_{k\sigma}(t), a^\dagger_{k\sigma}(0) \} \rangle, \quad D(k\omega) = -i\theta(\omega) \langle [s^z_k(t), s^z_{-k}] \rangle,$$

where angular brackets denote canonical ensemble averaging, $a_{k\sigma} = N^{-1/2} \sum_n \exp(-ikn) a_{n\sigma}$ and $s^z_k = N^{-1/2} \sum_n \exp(-ikn) s^z_n$ with the number of sites $N$. To calculate Green’s functions (2) we use their continued fraction representation [3, 4],

$$\langle \langle A_0 | A^\dagger_0 \rangle \rangle_\omega = \frac{|A_0 \cdot A^\dagger_0|}{\omega - E_0 - \frac{F_0}{\omega - E_1 - \frac{F_1}{\ddots}}}$$

where $\langle \langle A_0 | A^\dagger_0 \rangle \rangle_\omega$ is the Fourier transformation of one of the above Green’s functions and the operator $A_0$ is equal to $a_{k\sigma}$ or $s^z_k$. The coefficients $E_i$ and $F_i$ of continued fraction (3) are determined by the recursive procedure

$$[A_n, H] = E_n A_n + A_{n+1} + F_{n-1} A_{n-1},$$

$$E_n = [A_n, H] \cdot A^\dagger_n |A_n \cdot A^\dagger_n|^{-1}, \quad F_{n-1} = |A_n \cdot A^\dagger_n| A_{n-1} \cdot A^\dagger_{n-1} |^{-1}.$$

The definition of the inner product $|A \cdot B^\dagger|$ depends on the considered function. In the case of the anticommutator Green’s function $G(k\omega)$ in Eq. (2)
this inner product is defined as $\langle [A, B^\dagger] \rangle$, while for the commutator function $D(k\omega)$ it is $\langle [A, B^\dagger] \rangle$. However, in this latter case for the particular operator $A_0 = s_k^z$ the numerator of the continued fraction in Eq. (3) vanishes. Therefore the direct application of Eqs. (3) and (4) for the calculation of $D(k\omega)$ is impossible. Instead we consider Kubo’s relaxation function

$$
(s_k^z s_{-k}^z)_{t} = \theta(t) \int_{t}^{\infty} dt' \langle [s_k^z(t'), s_{-k}^z] \rangle.
$$

Continued fraction representation (3) with recursive procedure (4) is also valid for this relaxation function, if the inner product is defined as $\langle A, B^\dagger \rangle = i \int_{0}^{\infty} dt \exp(-\eta t)\langle [A(t), B^\dagger] \rangle$, $\eta \to +0$. On calculating the relaxation function, Green’s function is found from the relation

$$
\omega \langle (s_k^z s_{-k}^z) \rangle = \langle (s_k^z s_{-k}^z) \rangle + (s_k^z s_{-k}^z).
$$

For reasons of space we shall not go into details of the calculations and give only final results (a more detailed discussion will be published elsewhere). The spin Green’s function reads

$$
D(k\omega) = \frac{2\omega (s_k^z s_{-k}^z) \Pi(k\omega) + 4JC_1(\gamma_k - 1)}{\omega^2 - 2\omega \Pi(k\omega) - \omega_k^2},
$$

with the square of the frequency of magnetic excitations

$$
\omega_k^2 = 16J^2\alpha |C_1|(1 - \gamma_k)(\Delta + 1 + \gamma_k)
$$

and the imaginary part of the polarization operator

$$
\text{Im} \Pi(k\omega) = \pi \frac{\omega}{\omega} \sum_{k'} f_{k'k}^2 \int_{-\infty}^{\infty} d\omega' [n_F(\omega') - n_F(\omega' - \omega)]
\times A(k' - k, \omega' - \omega) A(k'\omega')
$$

(the real part of $\Pi(k\omega)$ is determined from the dispersion relations). In the above equations, $(s_k^z, s_{-k}^z)^{-1} = 4J\alpha(\Delta + 1 + \gamma_k)$, $\Delta = C_2/|C_1| + (1 - \alpha)/(8\alpha |C_1|) - 3/4$, $\gamma_k = \frac{[\cos(k_x) + \cos(k_y)]}{2}$, $n_F(\omega) = \exp(\omega/T) + 1)^{-1}$, $T$ is the temperature, $f_{k'k} = 2tN^{-1/2}(\gamma_{k'} - \gamma_{k'} - k)(s_k^z, s_{-k}^z)^{-1/2}$, and the hole spectral function $A(k\omega) = -\pi \text{Im} G(k\omega)$. The parameters $C_p = N^{-1} \sum_k \gamma_k^p C_k$ with $p = 1, 2$ and $C_k = \sum_n \exp[i k(n - m)](s_n^z, s_{-n}^z)$ appear in the above formulas after the decoupling of correlations containing four spin operators. These correlations arise in the second step of recursive procedure (4) and the decoupling serves as the terminator for continued fraction (3). Following Ref. [5] we somewhat improve this approximation by multiplying the result of the decoupling with the vertex correction $\alpha$. 
The parameters $C_1$, $C_2$ and $\alpha$ are calculated from the above definition of $C_p$ and the constraint of zero site magnetization in the paramagnetic state,

$$\langle s^+_n \rangle = \frac{1}{2} (1 - x) - \langle s^{-1}_n s^{+1}_n \rangle = 0,$$

which can be written in the form $N^{-1} \sum_k C_k = 1/2$ for small hole concentrations $x = \langle X_n \rangle$. In this equation and in $C_p$ the value of $C_k$ is determined by the equation

$$C_k = 4J|C_1|(1 - \gamma_k)\omega_k^{-1} \coth[\omega_k/(2T)],$$

which follows from Eq. (7).

The parameter $\Delta$ describes a gap near the point $(\pi, \pi)$ of the Brillouin zone in excitation spectrum (8). As follows from our calculations, the gap opens at $x \approx 0.01$ for $T = 0$ and, in accord with the Mermin-Wagner theorem [6], for any nonzero $T$. The gap opening indicates the destruction of the long-range antiferromagnetic order and the establishment of the short-range order with the correlation length which is determined by the gap magnitude. Notice that Eq. (9) is close in its form to the polarization operator obtained in Ref. [2] for the same model in the spin-wave approximation. However, the effective interaction constant $f^2_{k,k'}\omega^{-1}_k$ differs somewhat from the constant of the spin-wave approximation.

As can be shown by analogous calculations of the transversal spin Green’s function $D_\perp(kt) = -i\theta(t)\langle s^{-1}_k(t)s^{+1}_k \rangle$,

$$D_\perp(kt) = 2D(kt),$$

as it has to be in the paramagnetic state. Thus, the approximations made do not violate the rotation symmetry of the solution. Equation (12) was used in the derivation of Eq. (11).

The hole Green’s function reads

$$G(k\omega) = \phi[\omega - \varepsilon_k - \mu - \Sigma(k\omega)]^{-1},$$

where $\phi = (1 + x)/2$, the unrenormalized hole energy for moderate $x$

$$\varepsilon_k \approx \left(1 - 4\alpha^2C^2_1 + 4C_1 \right) \phi^{-1}t\gamma_k,$$

and the imaginary part of the hole self-energy

$$\text{Im} \Sigma(k\omega) = \pi \sum_{k'} h_{kk'} \int_{-\infty}^{\infty} d\omega' \left[ n_B(\omega') + n_F(\omega - \omega') \right]$$

$$\times A(k - k', \omega - \omega') B(k'\omega'),$$

which follows from Eq. (7).
Figure 1. The spin correlations \( Z(l) = 4|\langle s_{l(0)}^z s_{(0,0)}^z \rangle | \) calculated for \( T/J = 0.5, 0.75 \) and 1 in this work (open circles) and by the Monte Carlo method in Ref. [7] (filled circles). In both calculations a 32×32 lattice without holes was used.

Figure 2. The hole spectral function \( A(k_\omega) \) for the case of one hole in a 4×4 lattice, \( k = (\pi/2, \pi/2) \) and parameters \( J = 0.2t, \eta = 0.1t \). Our calculations for \( T = 0.02t \) and zero-temperature exact-diagonalization data of Ref. [8] are given in panels (a) and (b), respectively.

with \( h_{kk'} = 32(N\phi)^{-1}t^2 \{ (\gamma_k - \gamma_{k'})^2 + (\gamma_k^2 - \gamma_{k'}^2)[(1 + \gamma_{k'})/(1 - \gamma_{k'})]^{1/2} \} \), \( n_B(\omega) = [\exp(\omega/T) - 1]^{-1} \) and the spin spectral function \( B(k_\omega) = -\pi^{-1} \text{Im } D(k_\omega) \). It may be noticed that the general structure of Eq. (15) coincides with the respective equation in the spin-wave approximation [2] where the interaction constant is close to \( h_{kk'} \). From Eq. (11) for an infinite lattice and small \( x \) and \( T \) we find \( C_1 = -0.206734 \) and \( \alpha = 1.70494 \) (this value of \( C_1 = \langle s_{n}^{-1}s_{m}^{-1} \rangle \) with \( n \) and \( m \) being nearest neighbors is close to the value obtained in Monte Carlo simulations [7]). With these parameters \( \varepsilon_k \approx -0.65t\gamma_k \). Thus the width of the unrenormalized band is much smaller
The hole spectral function along the $(0,0) - (\pi,0)$ direction of the Brillouin zone. The calculations were carried out on a $20 \times 20$ lattice for the parameters $t = 0.5$ eV, $J = 0.1$ eV, $x \approx 0.1$ and $T = 0$. The Fermi energy is taken as zero of energy. In contrast to Fig. 2 the electron picture is used in this figure.

than the bandwidth in the absence of correlations when the dispersion is described by $4t\gamma_k$. This difference stems from the antiferromagnetic alignment of spins which leads to spin flipping accompanying the hole motion.

To check the validity of the approximations made we carried out a number of calculations which allowed comparison with exact diagonalisation and Monte Carlo data. In Fig. 1 results of our calculations of the spin correlations are compared with Monte Carlo data of Ref. [7]. In Fig. 2 the hole spectral function $A(k\omega)$ obtained from our calculations and by exact diagonalization in Ref. [8] are compared. In both calculations the artificial broadening $\eta = 0.1t$ was introduced to transform $\delta$-functions into Lorentzians. As is seen from these figures, our calculations are in good agreement with the numerical experiments.

The mentioned similarity of Eqs. (7), (9), (13) and (15) to the respective equations of the spin-wave approximation [2] at moderate doping leads to close resemblance in shape of the spectral functions obtained in these two approaches. As an example of the obtained results, the hole spectral function is shown in Fig. 3 for values of $t$ and $J$ which correspond to parameters of cuprate perovskites. As seen from the figure, for moderate doping the hole spectrum contains two dispersive features for wave vectors near the boundary of the magnetic Brillouin zone. One of these features – a narrow
intensive peak slightly below (in the electron picture) the Fermi level $\omega = 0$ – is connected with the so-called spin-polaron band. In a lightly doped crystal the width of this band is of the order of the exchange constant $J$ which is much smaller than the hopping constant $t$ for parameters of cuprate perovskites. The spin-polaron bandwidth is characterized by the parameter of magnetic excitations because on the antiferromagnetic background the hole movement is accompanied by spin flipping. The short-range antiferromagnetic ordering is retained in moderately doped crystals. In these conditions a part of the spin-polaron band is preserved near the boundary of the magnetic Brillouin zone. The second dispersive feature is a broad maximum the dispersion of which is characterized by the second energy parameter of the model $t$. The shape of this dispersion reproduces with some distortion the shape of the two-dimensional nearest-neighbor band. For wave vectors near the $\Gamma$ point two broad maxima, one below and one above the Fermi level, are seen in Fig. 3. Both of them belong to the dispersion with the characteristic energy $t$.

The Fermi surface derived from the spectral functions in the underdoped case is shown in Fig. 4a. The solid segments along the boundary of the magnetic Brillouin zone are formed by points where the spin-polaron band touches the Fermi level (notice that this band does not cross it). The Fermi level is crossed by the broader dispersive feature along the dashed curves. The spectral functions calculated for wave vectors on these curves are shown in Fig. 4b. On moving from $(\pi/2, \pi/2)$ to $(\pi/5, \pi)$ on the boundary of the Brillouin zone the spin-polaron peak recedes from the Fermi level. The situation looks like no Fermi level crossing occurs near $(\pi/5, \pi)$ and a gap opens between the energy band and the Fermi level. Only on another scale (compare Fig. 2) one can see that in this region the Fermi level crossing does exist. It is not seen in Fig. 4b because the maximum which crosses the Fermi level is completely lost at the foot of the more intensive spin-polaron peak and this peak is positioned somewhat below the Fermi level. Analogous behavior of the photoemission leading edge is observed in cuprate perovskites and is known as the photoemission pseudogap [9, 10]. Notice that the shape of the photoemission spectrum is determined by the spectral function and the correlation between their behaviors is expected. In Fig. 4c the positions of the spin-polaron peak in the spectral functions and the leading edge of the photoemission spectrum measured [9] in underdoped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ are compared for wave vectors on the Fermi surface. The magnitude of the pseudogap calculated for $x = 0.121$ and its symmetry are close to those observed experimentally. Moreover, at $x = 0.171$ which is close to the optimal doping concentration the calculated pseudogap disappears. This is also in agreement with experiment.

Two distinct emissions were observed recently in the normal state pho-
Figure 4. (a) The Fermi surface for the underdoped case. (b) The hole spectral functions for wave vectors on the dashed curve of the Fermi surface in panel (a). Curves from top to bottom correspond to $\mathbf{k} = (0.2\pi, \pi), (0.2\pi, 0.9\pi), (0.2\pi, 0.8\pi), (0.3\pi, 0.7\pi), (0.4\pi, 0.6\pi)$ and $(0.5\pi, 0.5\pi)$, respectively. $T = 116$ K, $x = 0.121$, $t = 0.5$ eV, and $J = 0.1$ eV. (c) The energy gap between the spin-polaron peak and the Fermi level along the dashed curve of the Fermi surface for $x = 0.121$ (squares) and $x = 0.171$ (diamonds) at $T = 116$ K. The position of the leading edge of the photoemission spectrum measured [9] in underdoped Bi$_2$Sr$_2$CaCu$_2$O$_6+\delta$ along the similar Fermi surface is indicated by filled circles.

toemission of the optimally doped Bi$_2$Sr$_{2-x}$La$_x$CuO$_{6+\delta}$ in the vicinity of the point $(\pi, 0)$ [11]. This crystal is a single CuO$_2$ layer material with sufficiently decoupled layers. Therefore the two emissions cannot be ascribed to the bilayer splitting. As mentioned, the hole spectral function of the two-dimensional $t$-$J$ model has also two components and it is reasonable to compare them with experimental data. The photoemission spectrum in Fig. 5(b) was obtained from the spectral function by convoluting it with a Gaussian to model experimental resolution and cutting off with the Fermi distribution. In accord with experimental conditions of Ref. [11], the Gaussian width 20 meV and the temperature 45 K were selected. In spite of some differences in relative intensities and widths of the spectral features, the calculated spectrum has the same structure as the experimental spec-
Figure 5. (a) The normal state photoemission spectrum of the optimally doped Bi$_{2}$Sr$_{2-\delta}$La$_{\delta}$CuO$_{6+\delta}$ ($T_c = 29$ K) at $T = 45$ K and $k = (0.62\pi, 0)$ [11]. (b) The photoemission spectrum calculated from the spectral function of the $t$-$J$ model for $t = 0.5$ eV, $J = 0.1$ eV, $x \approx 0.1$, $T = 45$ K and $k = (0.6\pi, 0)$. (c) The dispersions of the two features in the photoemission spectrum of Bi$_{2}$Sr$_{2-\delta}$La$_{\delta}$CuO$_{6+\delta}$ [11]. (d) The dispersions of the maxima in the spectral function in Fig. 3.

trum shown in panel (a). As in experiment, the maximum with a larger binding energy has a considerably larger width and stronger dispersion in comparison with the maximum with a lower binding energy. The experimental and calculated dispersions of the two spectral features are compared in panels (c) and (d). As is seen from the figure, they are similar and the binding energies are of the same order of magnitude. Recently two dispersive features were also resolved in the normal-state photoemission of the underdoped and optimally doped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ with two CuO$_2$ planes in the unit cell [12]. This splitting was connected with a coupling between the adjacent CuO$_2$ planes. Since energy distribution curves and values of the band splitting in that work are similar to those observed in the single CuO$_2$ plane material Bi$_{2}$Sr$_{2-\delta}$La$_{\delta}$CuO$_{6+\delta}$, another possible mechanism of the band splitting in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ – the above-discussed peculiarity of the spectrum of the two-dimensional strongly correlated system – has to be also taken into account. It counts in favour of this latter mechanism that the Fermi surface obtained in Ref. [12] (see Fig. 1g there) is very close to the Fermi surface in Fig. 4a.

In summary, the $t$-$J$ model of the CuO$_2$ plane was investigated with
the method which retains the rotation symmetry of the paramagnetic state and accounts properly for the kinematic interaction. The observed unusual properties of cuprates – the photoemission pseudogap and the band splitting – were shown to be inherent in the two-dimensional strongly correlated electron system.

Acknowledgements

This work was partially supported by the ESF grant No. 4022 and by the WTZ grant (Project EST-003-98) of the BMBF.

References

1. Izyumov, Yu.A. (1997) Strongly correlated electrons: the $t$-$J$ model, Phys.-Usp. (Russia) 40, 445-476.
2. Sherman, A. and Schreiber, M. (1999) Pseudogaps and magnetic properties of the two-dimensional $t$-$J$ model, in Narlikar, A.V. (ed.), Studies of High Temperature Superconductors, vol. 27, Nova Science Publishers, New York, pp. 163-187; cond-mat/9808087.
3. Mori, H. (1965) A continued-fraction representation of the time-correlation functions, Progr. Theor. Phys. 34, 399-416.
4. Sherman, A.V. (1987) A modified Lanczos algorithm and the continued-fraction representation of correlation functions. An example: a correlation function of the electron-phonon system, J. Phys. A 20, 569-576.
5. Kondo, J. and Yamaji, K. (1972) Green’s function formalism of the one-dimensional Heisenberg spin system, Progr. Theor. Phys. 47, 807-818.
6. Mermin, N.D. and Wagner, H. (1966) Absence of ferromagnetism or antiferromagnetism in one- or two-dimensional isotropic Heisenberg models, Phys. Rev. Lett. 17, 1133-1136.
7. Makivić, M.S. and Ding, H.-Q. (1991) Two-dimensional spin-$\frac{1}{2}$ Heisenberg antiferromagnet: a quantum Monte Carlo study, Phys. Rev. B 43, 3562-3574.
8. Dagotto, E., Joynt, R., Moreo, A., Bacci, S., and Gagliano, E. (1990) Strongly correlated electronic systems with one hole: dynamical properties, Phys. Rev. B 41, 9049-9073.
9. Ding, H., Yokoya, T., Campuzano, J.C., Takahashi, T., Randeria, M., Norman, M.R., Mochiku, T., Kadowaki, K., and Giapintzakis, J. (1996) Spectroscopic evidence for a pseudogap in the normal state of underdoped high-$T_c$ superconductors, Nature 382, 51-54.
10. Damascelli, A., Lu, D.H., and Shen, Z.-X. (2001) From Mott insulator to overdoped superconductor: evolution of the electronic structure of cuprates studied by ARPES, J. Electron Spectr. Relat. Phenom. 117-118, 165-187.
11. Janowitz, C., Müller, R., Dudy, L., Kräpf, A., Manzke, R., Ast, C., and Höchst, H. (2001) Unusual electronic ground state of a prototype cuprate: band splitting of single CuO$_2$ plane Bi$_2$Sr$_{2-x}$La$_x$CuO$_{6+δ}$, cond-mat/0107089.
12. Chuang, Y.-D., Gromko, A.D., Fedorov, A.V., Aiura, Y., Oka, K., Ando, Y., and Dessau, D.S. (2001) Constancy of the bilayer splitting as a function of doping in Bi$_2$Sr$_2$CaCuO$_{6+δ}$, cond-mat/0107002.
Energy (eV)

A

(\pi,0)

(0,0)

k

Energy (eV)
