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1998 J. Phys.: Condens. Matter 10 8007

(http://iopscience.iop.org/0953-8984/10/36/011)

J. Phys.: Condens. Matter **10** (1998) 8007–8014. Printed in the UK PII: S0953-8984(98)94241-2

Theory of the spin polaron in the t–J model

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Received 13 May 1998, in final form 14 July 1998

Abstract. A fully analytical theory is developed for the motion of a single hole in the t–J model based on the spin-polaron idea. With a self-consistent treatment of the hole–spin-wave interaction, we are able to overcome the difficulties encountered by the intermediate-coupling theory of Barentzen and obtain a theory applicable over the full range of the coupling strength. Good agreement with numerical studies is achieved.

The problem of hole motion in an antiferromagnetic background has become one of the central issues in developing the theory of high-temperature superconductivity, since the undoped parent phases of copper oxide materials are antiferromagnetic insulators. The t–J model is the simplest and most frequently used model for describing such strongly correlated systems. Numerous authors have studied this problem within the t–J model description [1–12], both analytically and numerically. Although there has been increasing consensus concerning the bandwidth, band shape and spectral weight of the coherent motion of the doped hole [13], the situation is still controversial, largely due to the fact that most of these studies rely on numerical calculation for small clusters (even the self-consistent Born approximation theory (SCBA) involves solving Dyson's equation for a small cluster [9]) and cannot be extended to the thermodynamic limit. Hence a fully analytical theory is highly desirable.

Intuitively, one expects the moving hole in the t–J model to be dressed by a cloud of virtual spin excitations, in much the same way as an electron in a polar crystal is dressed by virtual phonons [14]. In view of this formal similarity, it is natural to treat this problem using the methods of polaron theory. Along these lines, Barentzen has put forward an analytical theory [8] with the aid of the intermediate-coupling treatment of Lee, Low and Pines for the Fröhlich polaron problem [15]. But, as pointed out by Barentzen, such an intermediate-coupling theory is inapplicable in the strong-coupling regime which is of physical interest. For example, it predicts a monotonically increasing bandwidth as a function of the coupling strength t/J and finite limiting values for both the bandwidth (of order t) and the spectral weight in the strong-coupling limit. It is also found that this theory produces an artificial gap in the spin-excitation spectrum which grows with increasing coupling strength upon doping an additional hole into the antiferromagnetic background, and it has been argued that this may be why intermediate-coupling theory fails in the strong-coupling regime. Furthermore, we note that the result of this theory is a set of coupled integral equations whose solution also relies on numerical calculation for a finite momentum cluster, and we can hardly gain any useful intuition about the motion of the hole from such a complicated calculation.

In this article, we put forward a fully analytical theory for the motion of a single hole in the t–J model based on the spin-polaron idea. With a self-consistent treatment of the

0953-8984/98/368007+08$19.50

hole–spin-wave interaction, we are able to overcome the difficulties encountered by the intermediate-coupling theory and thus obtain a theory applicable over the whole range of the coupling strength. We find that at the weak-coupling limit ($t/J \ll 1$), the hole band has a width of order t^2/J and the spectral weight of the coherent motion of the hole approaches unity, while in the strong-coupling limit ($t/J \gg 1$), the bandwidth behaves as $J\ln(t/J)$ and the corresponding spectral weight vanishes like J/t. Furthermore, we find that the band shape evolves monotonically between these two limiting cases with the coupling strength t/J. In the weak-coupling regime (when $t/J < 0.675$), the band minimum is located at $(\pi/2, \pi/2)$ with a shallow hole pocket around it, and $(\pi, 0)$ is quasi-degenerate with the band minimum and is surrounded by an extended flat region. However, in the strong-coupling regime (when $t/J > 0.675$), the band minimum is replaced by $(\pi, 0)$, and $(\pi/2, \pi/2)$ becomes a saddle point. A possible relation to a result from a recent photoemission experiment is addressed.

In the linear spin-wave approximation, the Hamiltonian of the t–J model reads [3, 4]

$$H = \sum_{\boldsymbol{q}} \omega_{\boldsymbol{q}} b_{\boldsymbol{q}}^{\dagger} b_{\boldsymbol{q}} + \frac{zt}{\sqrt{N}} \sum_{\boldsymbol{k},\boldsymbol{q}} [M_{\boldsymbol{q}}(\boldsymbol{k}) f_{\boldsymbol{k}-\boldsymbol{q}}^{\dagger} f_{\boldsymbol{k}} b_{\boldsymbol{q}}^{\dagger} + \text{HC}] \tag{1}$$

where

$$\omega_{\boldsymbol{q}} = \frac{zJ}{2}\omega(\boldsymbol{q}) \qquad \omega(\boldsymbol{q}) = \sqrt{1-\gamma_{\boldsymbol{q}}^2}$$

$$M_{\boldsymbol{q}}(\boldsymbol{k}) = u_{\boldsymbol{q}}\gamma_{\boldsymbol{k}-\boldsymbol{q}} + v_{\boldsymbol{q}}\gamma_{\boldsymbol{k}} \qquad \gamma_{\boldsymbol{q}} = \frac{1}{z}\sum_{\boldsymbol{d}} \exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{d}).$$

Here $f_{\boldsymbol{k}}$ and $b_{\boldsymbol{q}}$ are the annihilation operators of the hole and spin waves, $\boldsymbol{d}$ denotes the nearest-neighbouring bond vector, and $u_{\boldsymbol{q}}$ and $v_{\boldsymbol{q}}$ are the usual Bogoliubov transformation coefficients:

$$u_{\boldsymbol{q}} = \sqrt{\frac{1+\omega(\boldsymbol{q})}{2\omega(\boldsymbol{q})}} \qquad v_{\boldsymbol{q}} = -\text{sgn}(\gamma_{\boldsymbol{q}})\sqrt{\frac{1-\omega(\boldsymbol{q})}{2\omega(\boldsymbol{q})}}.$$

Obviously, the total momentum of the hole and the spin-wave system is a constant of the motion. As in the polaron problem, we introduce a unitary transformation U to eliminate the momentum of the spin-wave system so as to partially diagonalize the Hamiltonian with respect to the hole operator. For the single-hole problem, U is given by [8, 16]

$$U = \sum_{\boldsymbol{k},\boldsymbol{p}} \left(\frac{1}{N}\sum_i T_i \mathrm{e}^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{R}_i}\right) f_{\boldsymbol{k}}^{\dagger} f_{\boldsymbol{k}-\boldsymbol{p}} \tag{2}$$

where

$$T_i = \exp\left(-\mathrm{i}\boldsymbol{R}_i \cdot \sum_{\boldsymbol{q}} \boldsymbol{q} b_{\boldsymbol{q}}^{\dagger} b_{\boldsymbol{q}}\right)$$

is the translation operator for the boson field. The transformed Hamiltonian now takes the form

$$U^{\dagger}HU = \sum_{\boldsymbol{k}} H_{\boldsymbol{k}} f_{\boldsymbol{k}}^{\dagger} f_{\boldsymbol{k}} \tag{3}$$

in which

$$H_{\boldsymbol{k}} = \sum_{\boldsymbol{q}} \omega_{\boldsymbol{q}} b_{\boldsymbol{q}}^{\dagger} b_{\boldsymbol{q}} + \frac{zt}{\sqrt{N}} \sum_{\boldsymbol{q}} [\Gamma_{\boldsymbol{q}}(\boldsymbol{k}) b_{\boldsymbol{q}} + \text{HC}] \tag{4}$$

where

$$\Gamma_{q}(\boldsymbol{k}) = u_{q}\Gamma_{k-q} + v_{q}\Gamma_{k} \qquad \Gamma_{k} = \frac{1}{z}\sum_{d} T_{d}\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{d}).$$

Here H_k represents the Hamiltonian for momentum $\boldsymbol{k}$. It looks just like the Hamiltonian for a group of displaced harmonic oscillators except that the external force $\Gamma_q(\boldsymbol{k})$ now depends on the displacement itself. In the following, we replace $\Gamma_q(\boldsymbol{k})$ by its expectation value $\langle\Gamma_q(\boldsymbol{k})\rangle$ in the ground state and determine it self-consistently. Unlike in the ordinary mean-field decoupling procedure, here we have neglected the fluctuation in $\Gamma_q(\boldsymbol{k})$. However, if we treat the second term in equation (4) as a perturbation, then $\langle b_q\rangle$ is of higher order than $\langle\Gamma_q(\boldsymbol{k})\rangle$, so our decoupling procedure is justified when $\langle b_q\rangle$ is small. As we will see below (from equation (5) and equation (10)), $\langle b_q\rangle$ is proportional to t/J, so our approximation is justified when t/J is small. When t/J is large, the fluctuation in $\Gamma_q(\boldsymbol{k})$ may drastically change the dispersion. However, our results show good agreement with numerical work even in this regime. Making use of the following displacement transformation:

$$\bar{b}_{q} = b_{q} + \frac{zt}{\sqrt{N}}\frac{\langle\Gamma_{q}(\boldsymbol{k})\rangle}{\omega_{q}} \tag{5}$$

H_k can be diagonalized as

$$H_{k} = \sum_{q}\omega_{q}\bar{b}^{\dagger}_{q}\bar{b}_{q} + E_{0}(\boldsymbol{k}). \tag{6}$$

Here $E_0(\boldsymbol{k})$ denotes the ground-state energy of the single-hole system with total momentum $\boldsymbol{k}$, i.e., the dispersion relation of the hole motion. It reads

$$E_{0}(\boldsymbol{k}) = -\frac{(zt)^{2}}{N}\sum_{q}\frac{\langle\Gamma_{q}(\boldsymbol{k})\rangle^{2}}{\omega_{q}}. \tag{7}$$

The ground state of the spin-wave system is the following coherent state of b_q-operators:

$$|\Psi_{k}\rangle = \exp\!\left(-\frac{(zt)^{2}}{2N}\sum_{q}\frac{\langle\Gamma_{q}(\boldsymbol{k})\rangle^{2}}{\omega_{q}^{2}} - \frac{zt}{\sqrt{N}}\sum_{q}\frac{\langle\Gamma_{q}(\boldsymbol{k})\rangle}{\omega_{q}}b^{\dagger}_{q}\right)|0\rangle. \tag{8}$$

Unlike in the intermediate-coupling theory, in our self-consistent treatment, the spin-excitation spectrum is unaltered upon the doping of an additional hole into the antiferromagnetic background. We think that this is the key difference between our theory and the intermediate-coupling theory, and it explains why intermediate-coupling theory fails in the strong-coupling regime. Now $\langle\Gamma_q(\boldsymbol{k})\rangle$ can be evaluated self-consistently in $|\Psi_k\rangle$. It is determined by the following integral equation:

$$\langle\Gamma_{q}(\boldsymbol{k})\rangle = \frac{1}{z}\sum_{d}\exp\!\left(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{d} - \frac{(zt)^{2}}{N}\sum_{p}\frac{\langle\Gamma_{p}(\boldsymbol{k})\rangle^{2}}{\omega_{p}^{2}}(1-\mathrm{e}^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{d}})\right)(v_{q} + u_{q}\mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{d}}). \tag{9}$$

Making use of the symmetry property of $\langle\Gamma_q(k)\rangle$, namely

$$\langle\Gamma_{q+Q}(k)\rangle = -\langle\Gamma_{q}(k)\rangle(Q = (\pi,\pi))$$

this equation can be solved analytically. The solution is

$$\langle\Gamma_{q}(\boldsymbol{k})\rangle = \exp(-A(\boldsymbol{k}))M_{q}(\boldsymbol{k}). \tag{10}$$

$M_q(\boldsymbol{k})$ is defined by equation (1) and $A(\boldsymbol{k})$ is determined by the following equation:

$$A(\boldsymbol{k})\exp(2A(\boldsymbol{k})) = \frac{(zt)^{2}}{N}\sum_{q}\frac{M_{q}(\boldsymbol{k})^{2}}{\omega_{q}^{2}}. \tag{11}$$

Inserting equation (10) into equation (7), we arrive at the following expression for the dispersion relation:

$$E_0(\boldsymbol{k}) = -\frac{(zt)^2}{N}\exp(-2A(\boldsymbol{k}))\sum_{\boldsymbol{q}}\frac{M_{\boldsymbol{q}}(\boldsymbol{k})^2}{\omega_{\boldsymbol{q}}}. \tag{12}$$

Now we consider the spectral weight. By definition,

$$Z_{\boldsymbol{k}} = |\langle\phi_{\boldsymbol{k}}^{(0)}|\phi_{\boldsymbol{k}}\rangle|^2. \tag{13}$$

Here $|\phi_{\boldsymbol{k}}^{(0)}\rangle = f_{\boldsymbol{k}}^{\dagger}|0\rangle$ denotes the unperturbed ground state, while $|\phi_{\boldsymbol{k}}\rangle = U^{\dagger}f_{\boldsymbol{k}}^{\dagger}|\Psi_{\boldsymbol{k}}\rangle$ denotes the ground state of the full Hamiltonian. Using equation (2) and equation (8), it is fairly straightforward to show that

$$Z_{\boldsymbol{k}} = \exp(-A(\boldsymbol{k})). \tag{14}$$

We first consider the limiting cases. In the weak-coupling limit ($t/J \ll 1$), we have $A(\boldsymbol{k}) \to 0$, and, by equation (7),

$$E_0(\boldsymbol{k}) \approx -\frac{(zt)^2}{N}\sum_{\boldsymbol{q}}\frac{M_{\boldsymbol{q}}(\boldsymbol{k})^2}{\omega_{\boldsymbol{q}}}. \tag{15}$$

(We note that this expression is identical to that derived from the SCBA in the same limit [9].) Hence the bandwidth W is of order t^2/J, and the spectral weight $Z_{\boldsymbol{k}} \to 1$ in this limit. In the strong-coupling limit ($t/J \gg 1$), we have $A(\boldsymbol{k}) \sim \ln(t/J)$, and, by equation (7),

$$E_0(\boldsymbol{k}) \sim -\ln(t/J)\left(\sum_{\boldsymbol{q}}\frac{M_{\boldsymbol{q}}(\boldsymbol{k})^2}{\omega_{\boldsymbol{q}}^2}\right)^{-1}\sum_{\boldsymbol{q}}\frac{M_{\boldsymbol{q}}(\boldsymbol{k})^2}{\omega_{\boldsymbol{q}}}. \tag{16}$$

Hence the bandwidth is of order $J\ln(t/J)$ and the spectral weight vanishes like J/t in this limit. These findings are in qualitative agreement with both numerical studies [9, 10, 12] and other analytical studies [4] (see figure 2, later). For example, Lanczos diagonalization shows that W varies linearly with J for $0.1 < J < 0.5$ and $Z_{k=(\pi/2,\pi/2)} \approx 0.622J^{0.598}$ for $0.1 < J < 1$ (using t as the unit of energy) while SCBA calculation gives $W \approx 1.5J^{0.79}$ and $Z_{k=(\pi/2,\pi/2)} \approx 0.63J^{0.667}$ for $0.01 < J < 0.5$. In contrast, intermediate-coupling theory predicts a monotonically increasing bandwidth as a function of the coupling strength t/J and finite limiting values for both the bandwidth (of order t) and the spectral weight in the strong-coupling limit. This may be a consequence of the artificial spin gap produced by inconsistent treatment of the hole–spin-wave interaction in the earlier theory, which grows with increasing coupling strength t/J.

The evolution of the band shape with the coupling strength between these two limiting cases is displayed in figure 1. In the weak-coupling regime (when $t/J < 0.675$), the band minimum is located at $(\pi/2, \pi/2)$ and there is a shallow hole pocket around it. $(\pi, 0)$ is quasi-degenerate with the band minimum and around it is the much-discussed extended flat region (figure 1(a)). All of these findings are in good agreement with numerical studies [9–12] and other analytical work [7]. A recent photoemission experiment has also found indications of the existence of such quasi-degeneracy and a flat region around $(\pi, 0)$ [17], but we note that the experiment was carried out for conditions near those of the optimal doping regime, so the validity of the rigid-band picture and even the validity of the t–J model itself are somewhat questionable, and a photoemission experiment on the antiferromagnetic insulator $Sr_2CuO_2Cl_2$ shows that although the strong renormalization of the hole bandwidth can be well described by the t–J model, the band shape cannot. It was noted that the simple t–J model is not an adequate description of real materials, and that other perturbations (like the next-nearest-neighbour hopping term) are important in

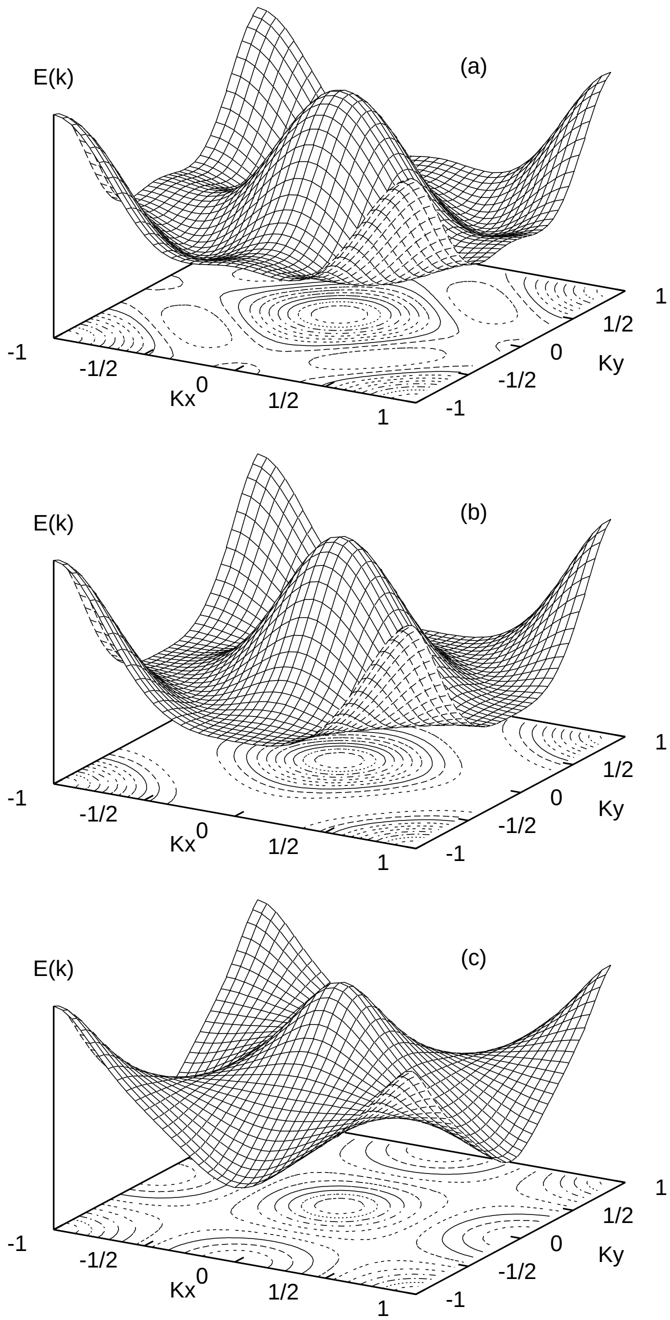

Figure 1. The evolution of the band shape with the coupling strength. (a) The weak-coupling limit. (b) t/J at the critical value 0.675. (c) The strong-coupling limit. $\boldsymbol{k}_x$ and $\boldsymbol{k}_y$ are in units of π.

determining the hole band shape. With the increase of the coupling strength, the energy at $(\pi, 0)$ decreases monotonically relative to the band minimum at $(\pi/2, \pi/2)$, and when t/J exceeds a critical value $(t/J)_c = 0.675$, the energy at $(\pi, 0)$ will be lower than that at

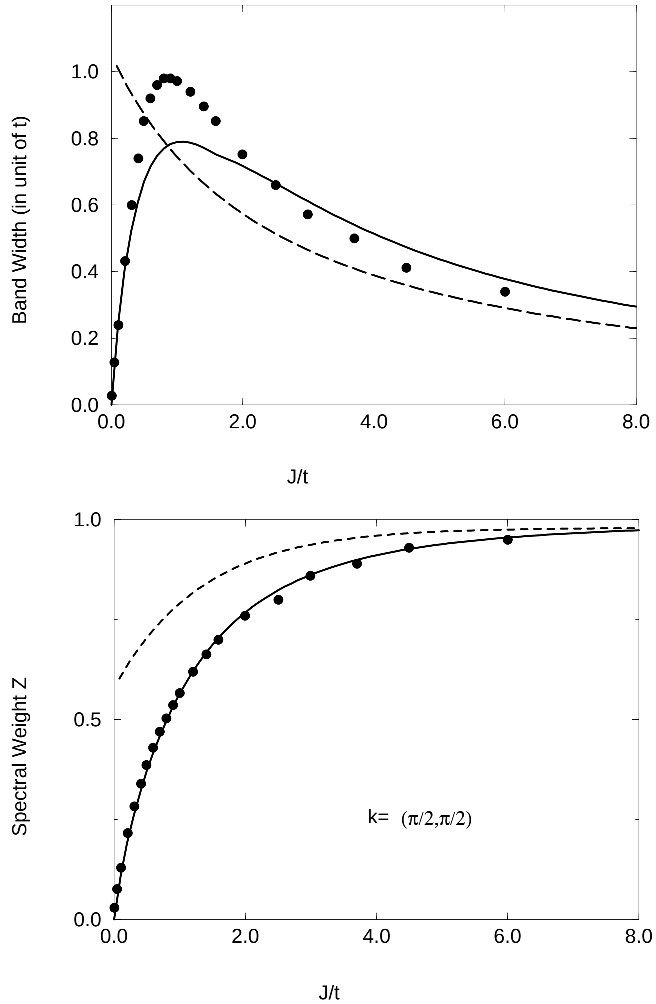

Figure 2. The bandwidth W and spectral weight $Z_{\boldsymbol{k}}$ as functions of J/t. Filled circles: the SCBA result based on a 16×16 lattice taken from reference [9]. Solid line: the result from our earlier theory. Dashed line: the result from the intermediate-coupling theory taken from reference [8]. The spectral weights are calculated at $\boldsymbol{k} = (\pi/2, \pi/2)$.

$(\pi/2, \pi/2)$, i.e., the band minimum will be replaced by $(\pi, 0)$. At the same time, $(\pi/2, \pi/2)$ will become a saddle point and the band shape will take on its strong-coupling-limit topology (see figures 1(b) and 1(c)). This observation is at variance with many previous results, and it may be an artifact of the present theory. However, we note that the problem of the location of the band minimum is a subtle one and the situation is still controversial.

To compare our theory with other studies more quantitatively, we show in figure 2 the bandwidth and the spectral weight given by our theory and those given by intermediate-coupling theory as compared with the results of a SCBA calculation based on a 16×16 lattice [9]. As can be seen from the figures, while the intermediate-coupling theory totally fails in the strong-coupling regime, our results are in good agreement with those obtained using the SCBA over the whole range of coupling strength, especially as regards the spectral weight, which is almost identical in the two theories. This further demonstrates

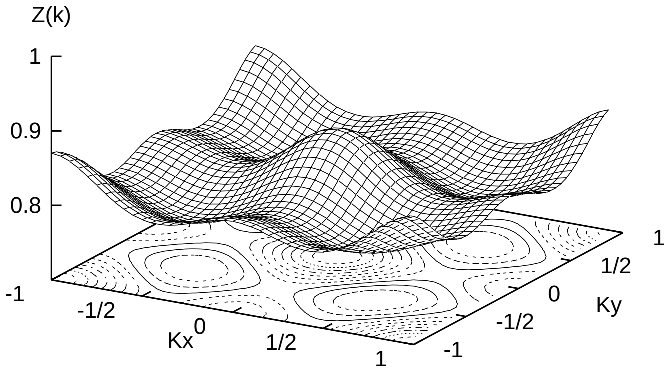

Figure 3. The variation of the spectral weight with momentum. The value of t/J is fixed at 1.

the reliability of our theory and the importance of a self-consistent treatment of the hole–spin-wave interaction. Finally, in figure 3 we display the variation of the spectral weight with momentum in the Brillouin zone for a fixed value of the coupling strength. Obviously, the spectral weight is a rather uniform function of the momentum. Its maximum is located at $(0, 0)$ and its minimum is located at $(\pi/2, \pi/2)$, irrespective of the coupling strength, contrary to the loop expansion result of reference [10].

In summary, we have developed a fully analytical theory for the motion of a single hole in the t–J model based on the spin-polaron idea. With a self-consistent treatment of the hole–spin-wave interaction, we are able to overcome the difficulties encountered by intermediate-coupling theory and hence obtain a theory applicable over the full range of the coupling strength. We find that the system can be classified into two regimes according to the location of the band minimum. In the weak-coupling regime ($t/J < 0.675$), the band minimum is located at $(\pi/2, \pi/2)$, with a shallow hole pocket around it. $(\pi, 0)$ is quasi-degenerate with the band minimum and there is an extended flat region around it. However, in the strong-coupling regime ($t/J > 0.675$), the band minimum is replaced by $(\pi, 0)$, and $(\pi/2, \pi/2)$ becomes a saddle point. In both regimes, the band maximum is located at $(0, 0)$. In the weak-coupling limit ($t/J \ll 1$), the bandwidth is of order t^2/J and the spectral weight approaches unity, while in the strong-coupling limit ($t/J \gg 1$), the bandwidth behaves as $J \ln(t/J)$ and the spectral weight vanishes like J/t.

Acknowledgments

One of us (TL) would like to thank Xing Yang and Xue-Ping Yu for valuable help.

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