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Spin-Polaron Wave Function for a Single Hole in an Antiferromagnet

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The wave function of a single hole moving in a two-dimensional antiferromagnet is derived from the Green's function obtained within self-consistent Born approximation. Starting from the wave function various correlation functions which characterize the distortion of the antiferromagnetic background around the hole can be calculated. Both the t-J and the t-J_z model are studied. Whereas for the $t - J_z$ model these perturbations are essentially isotropic and decay exponentially with the distance from the hole, their decay in the $t-J$ model has power-law form. Moreover the correlation functions in the $t - J$ model are are highly anisotropic and depend strongly on the momentum of the quasiparticle.

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1. Introduction

The Green's function for a hole moving in a *fixed* spin background has been discussed in the context of transition metal oxides in the late 60th by Bulaevskii et al[1] and by Brinkman and Rice.[2] In this case the Green's function is local and fully incoherent. The first prediction that the low-energy charge excitations in the 2D $t - J$ model[3]

$$H = -t \sum_{<ij>\sigma} \left(\tilde{c}^{\dagger}_{i,\sigma}\tilde{c}_{j,\sigma} + h.c.\right) + J \sum_{<ij>} [S^z_i S^z_j + \frac{\alpha}{2}(S^+_i S^-_j + S^-_i S^+_j)] \qquad (1)$$

are propagating quasiparticles with a bandwidth of order J was made by Kane, Lee and Read[4] and was confirmed by a number of exact diagonalization studies.[5,6] The problem is complicated due to the constraint on the fermion operators $\tilde{c}^{\dagger}_{i,\sigma} = c^{\dagger}_{i,\sigma}(1-n_{i,-\sigma})$ and by the fact that quantum fluctuations play a crucial role. This model has been widely studied particularly because it is considered to contain much of the low-energy physics of the high-T_c superconductors.[3,7] Nevertheless fundamental issues are still unclear such as the spin-dynamics and the form of the Fermi surface at moderate doping. Even in the case of a single hole there are different views e.g. whether the quasiparticle spectral weight is finite or vanishes in the thermodynamic limit. In particular Anderson has argued that holes introduce a deformation in the

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spin-background which decays as power law and as a consequence the spectral weight should vanish, — leading to non-Fermi liquid behaviour.[8]

We will describe here a slave fermion technique,[9,4] which was successful in reproducing the diagonalization results for the full Green's function.[6] The main aim of this work is to derive the wave function for the quasiparticle and to present a quantitative picture of the shape and size of the quasiparticle. Results of correlation functions describing the deformation of the spin-background around the hole will be presented for the t-J model ($\alpha = 1$ in Eq.(1)) as well as for the more simple t-J_z ($\alpha = 0$) model which has no spin-dynamics and a simple classical Néel ground state.

In a first step of the reformulation of the problem holes are described as spinless (slave) fermion operators, i.e. on the A sublattice a spinless fermion creation operator is defined as $h_i^+ = c_{i\uparrow}$ while the corresponding operator $c_{i\downarrow} = h_i^+ S_i^+$ is expressed as a composite operator, and similarly for the B-sublattice.[11] The kinetic energy then reads $H_t = -t\sum_{i,j(i)}(h_i h_j^+ S_j^- + \text{h.c.})$, that is, each hop of the fermion is connected with a spin-flip. The spin dynamics is described within linear spin wave theory (LSW) which provides a satisfactory approximation for the 2D spin-1/2 Heisenberg antiferromagnet. After performing the usual steps, i.e. Holstein-Primakoff, i.e. $S_i^+ \sim a_i$, and Bogoliubov transformation, the $t - J$ Hamiltonian takes the form:

$$H_{t-J} = \frac{1}{\sqrt{N}}\sum_{\mathbf{kq}}(M_{\mathbf{kq}} h^\dagger_{\mathbf{k}-\mathbf{q}} h_{\mathbf{k}} \alpha^\dagger_{\mathbf{q}} + \text{H.c.}) + \sum_{\mathbf{q}} \omega_{\mathbf{q}} \alpha^\dagger_{\mathbf{q}} \alpha_{\mathbf{q}}. \tag{2}$$

Here $\alpha_q = u_q a_q - v_q a^+_{-q}$ and $\omega_q = szJ\sqrt{1-\gamma_q^2}$ are the spin wave annihilation operator and energy, $\gamma_q = \frac{1}{2}(\cos q_x + \cos q_y)$ and $u_q(v_q)$ are the usual Bogoliubov coherence factors.[11] The kinetic energy in (1) appears now as the coupling term to the spin waves with the matrix element given by $M_{\mathbf{kq}} = 4t(u_{\mathbf{q}}\gamma_{\mathbf{k}-\mathbf{q}} + v_{\mathbf{q}}\gamma_{\mathbf{k}})$. Otherwise (2) is similar to the small polaron Hamiltonian except that a kinetic energy term for the spinless fermions is absent. As for the copper oxides $t > J$ this is a strong coupling problem and a selfconsistent technique is required.

The selfconsistent Born approximation for the fermion (holon) Green's function

$$G_{\mathbf{k}}(E) = \frac{1}{E - \Sigma_{\mathbf{k}}(E)} \tag{3}$$

amounts to the summation of all noncrossing diagrams. Here in contrast to the 'phonon' polaron problem vertex corrections turn out to be of minor importance.[11,12] The self-energy

$$\Sigma_{\mathbf{k}}(E) = \frac{1}{N}\sum_{\mathbf{q}} M^2_{\mathbf{k},\mathbf{q}} G_{\mathbf{k}-\mathbf{q}}(E - \omega_{\mathbf{q}}) \tag{4}$$

has to be solved selfconsistently. Typical numerical results for the spectral function $A(k,\omega) = -(1/\pi)\text{Im}G^h_{\mathbf{k}}(\omega)$ may be found in references [10-13]. The spectra show a bound state (quasiparticle) at low energy and a broad incoherent continuum of multi-magnon excitations distributed over an energy range of almost the free band width $W = 2zt$.

2. Quasiparticle Wave Function

Given the Green's function in selfconsistent Born approximation (scBA) it would be interesting to know the wave function of the quasiparticle which corresponds to the pole in (3) at energy $\epsilon_{\mathbf{k}} = \Sigma_{\mathbf{k}}(\epsilon_{\mathbf{k}})$. This wave function would allow us to calculate in principle all correlation functions which define the perturbation of the AF-background around the hole.

The quasiparticle wave function is the eigenstate of H

$$H\psi_{\mathbf{k}} = \epsilon_{\mathbf{k}}\psi_{\mathbf{k}}, \tag{5}$$

which gives rise to the quasiparticle peak with weight $Z_{\mathbf{k}}$ in the spectral representation for the Green's function (3)

$$\begin{aligned} G_{\mathbf{k}}(E) &= \sum_n \frac{|< \psi_{\mathbf{k}n} \mid h^+_{\mathbf{k}} \mid 0 >|^2}{E - E_{\mathbf{k}n}}, \\ &= \frac{Z_{\mathbf{k}}}{E - \epsilon_{\mathbf{k}}} + G^{inc}_{\mathbf{k}}(E). \end{aligned} \tag{6}$$

The spectral weight of the quasiparticle

$$Z_{\mathbf{k}} = |< \psi_{\mathbf{k}} \mid h^+_{\mathbf{k}} \mid 0 >|^2 \tag{7}$$

can be quite small, however it should not scale to zero in the thermodynamic limit, whereas the matrix elements contributing to the incoherent part are of O(1/N) or smaller.

In this section we present a derivation of the QP wave function ψ_k on the same level of approximation as the scBA for the Green's function. In particular we will prove that the QP weight derived from the wave function agrees with the result calculated directly from the selfenergy.

Given the Hamiltonian (2) we expect the wave function $\mid \psi_{\mathbf{k}} >$ to have the form

$$\begin{aligned} \mid \psi_k >= a^0(k)h^+_k|0> &+ \frac{1}{\sqrt{N}}\sum_{q_1} a^1(k,q_1)h^+_{k-q_1}\alpha^{+^{\circ}}_{q_1}|0> \\ &+ \frac{1}{N}\sum_{q_1q_2} a^2(k,q_1,q_2)h_{k-q_1-q_2}\alpha^+_{q_2}\alpha^+_{q_1}|0> \\ &+ \ \ldots\ldots\ldots \end{aligned} \tag{8}$$

where the coefficients $a^n(k,q_1,...,q_n)$ are to be determined. The state $|0>$ is the vacuum with respect to hole h_k amd spinwave operators α_q.

From the Schrödinger equation we obtain the following sequence of equations for the expansion coefficients:

$$Ea^0(k) - \frac{1}{N}\sum_{q_1} a^1(k,q_1)M_{kq_1} = 0 \tag{9}$$

$$(E-\omega_{q_1})a^1(k,q_1) - a^0(k)M_{k,q_1} - \frac{1}{N}\sum_{q_2} a^2(k,q_1,q_2)M_{k-q_1,q_2} = 0 \tag{10}$$

To obtain these equations which correspond to the noncrossing approximation for the Green's function one has to adopt the following contraction rule (CR): When one magnon is annihilated in the n-magnon component of the wave function (8) only the contribution is considered where the last magnon in the sequence, i.e. $\alpha^+_{q_n}$, is annihilated. This is reminescent of the retraceable path approximation in momentum space. The general equation for $n > 0$ reads:

$$(E - \omega_{q_1} ... - \omega_{q_n}) a^n(k, ..., q_n) - a^{n-1}(k, ..., q) M_{k_{n-1}, q_n} \\ - \frac{1}{N} \sum_{q_{n+1}} a^{n+1}(k, ..., q_{n+1}) M_{k_n, q_{n+1}} = 0, \qquad (11)$$

where $k_n = k - q_1 - ... - q_n$.

As first shown by Reiter[14] this sequence of equations (9-11) has the general solution

$$a^{n+1}(k, ..., q_{n+1}) = a^n(k, ..., q_n) M_{k_n, q_{n+1}} G_{k_{n+1}}(E - \omega_{q_1} - ... - \omega_{q_{n+1}}) . \qquad (12)$$

Substituting (12) into the last term on the *l.h.s.* of Eq. (11), we recognize that this term is identical to the expression (4) for the selfenergy Σ times a^n. This yields for (11)

$$(E - ... - \omega_{q_n} - \Sigma_{k_n}(E - ... - \omega_{q_n}))\, a^n(k, ..., q_n) - a^{n-1}(k, ..., q_{n-1}) M_{k_{n-1}, q_n} = 0 \qquad (13)$$

Since the prefactor of a^n is the inverse of the Green's function $G_{k_n}(E - \omega_{q_1} - ... - \omega_{q_n})$ this equation is identical to Eq. (12) with n replaced by $n - 1$. It only remains to be shown that also (9) is solved. Equation (9) becomes

$$a^0_k(E - \Sigma_k(E)) = 0 \, , \qquad (14)$$

which has a nontrivial solution $a^0_k \neq 0$ at the QP-energy $E = \epsilon_k$.

The knowledge of the Green's function (3) is sufficient to calculate from (12) iteratively the coefficients $a^n(k, q_1, ...q_n)$. The coefficient $a^0(k)$ which determines the QP-weight $Z_k = (a^0(k))^2$ follows from the normalization of the wave function

$$\begin{aligned} < \psi_k \mid \psi_k > &= \sum_{n=0}^{\infty} \mid a^n(k, ..., q_n) \mid^2 = 1 \\ &= (a^0(k))^2 \Big\{ 1 + \frac{1}{N} \sum_{q_1} (M_{k, q_1} G_{k-q_1}(\epsilon_k - \omega_{q_1}))^2 \\ &+ \frac{1}{N^2} \sum_{q_1 q_2} (M_{k q_1} G_{k-q_1}(\epsilon_k - \omega_{q_1}))^2 \cdot (M_{k-q_1, q_2} G_{k_2}(\epsilon_k - \omega_{q_1} - \omega_{q_2}))^2 \\ &+ \; ...... \Big\} \end{aligned} \qquad (15)$$

If one calculates the derivative $\partial\Sigma_k(E)/\partial E$ from Eq. (4) one recognizes that[15]

$$< \psi_k \mid \psi_k >= (a_k^0)^2 \cdot \left(1 - \frac{\partial \Sigma_k(E)}{\partial E}\right)_{E=\epsilon_k} . \tag{16}$$

As ψ_k is normalized to 1, this implies

$$Z_k = (a_k^0)^2 = \frac{1}{1 - \frac{\partial \Sigma_k(E)}{\partial E}} , \tag{17}$$

which is identical to the QP-spectral weight as calulated from G. This accomplishes the prove of the internal consistency of G and ψ. It should be emphasized that the above derivation does not rely on the assumption that the coupling term in the Hamiltonian is small.

3. Polaron in the $t - J_z$ Model

A first question one may ask is: "How many magnons are involved in the formation of the polaron". As the coupling between hole and spin-excitatitions is the kinetic energy of the t-J_z model, small values of J_z/t correspond to strong coupling, where many magnons will be excited. In order to estimate the number n of magnon terms needed in the wave function we have calculated the norm $\mathcal{N}_{\mathbf{k}}$

$$\mathcal{N}_{\mathbf{k}} = \langle \Psi_{\mathbf{k}}^{(n)} | \Psi_{\mathbf{k}}^{(n)} \rangle = \sum_{m=0}^{n} A_{\mathbf{k}}^{(m)} \tag{18}$$

as a function of J/t and for different n. The distribution $A_{\mathbf{k}}^{(m)}$ can be interpreted as a probability distribution that m magnons are excited in the wave function. According to Eq. (15) this distribution is given by

$$A_{\mathbf{k}}^{(m)} = \frac{Z_{\mathbf{k}}}{N^m} \sum_{\mathbf{q}_1,\ldots,\mathbf{q}_m} g_{\mathbf{k},\mathbf{q}_1}^2 g_{\mathbf{k}-\mathbf{q}_1,\mathbf{q}_2}^2 \cdots g_{\mathbf{k}-\mathbf{q}_1-\ldots,\mathbf{q}_m}^2 \tag{19}$$

where $g_{\mathbf{k},\mathbf{q}} = M_{\mathbf{kq}} G_{\mathbf{k}-\mathbf{q}}(\omega - \omega_{\mathbf{q}})$ with $\omega = \epsilon_{\mathbf{k}}$, and $A_{\mathbf{k}}^{(0)} \equiv Z_{\mathbf{k}}$

In the Ising limit of the model ($\alpha = 0$) the analysis becomes simple because the equations for the self-energy in scBA become independent on $\mathbf{k}$ and reduce to one equation $\Sigma_{\mathbf{k}}(\omega) = 4t^2[\omega - 2J - \Sigma_{\mathbf{k}}(\omega - 2J)]^{-1}$. This equation can then be expressed in a recurrence form

$$A_{\mathbf{k}}^{(m+1)} = A_{\mathbf{k}}^{(m)} [2tG_{\mathbf{k}}(\epsilon_{\mathbf{k}} - 2mJ)]^2. \tag{20}$$

In Fig. 1a the norm $\mathcal{N}_{\mathbf{k}}$ is shown for various n as a function of J/t.The crossover between the weak and the strong coupling regime may be located at $J/t \sim 0.3$. Below this value the number of magnon terms needed to fullfil the sum rule $\mathcal{N}_{\mathbf{k}} = 1$ increases dramatically. In Fig. 1b we present the distribution $A_{\mathbf{k}}^{(m)}$ for several values of J_z/t.

The average number of magnons can be calculated knowing $A_{\mathbf{k}}^{(m)}$

$$n_{mag} = \langle \Psi_{\mathbf{k}}^{(n)} | \sum_{\mathbf{q}} \alpha_{\mathbf{q}}^\dagger \alpha_{\mathbf{q}} | \Psi_{\mathbf{k}}^{(n)} \rangle = \sum_m m A_{\mathbf{k}}^{(m)}. \tag{21}$$

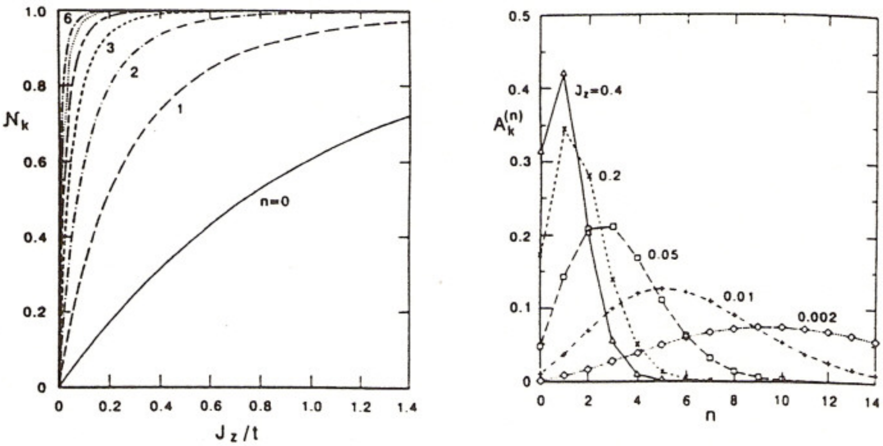

Fig. 1. (a) $\mathcal{N}_k$ versus J/t for the $t - J_z$ model, where n denotes the order of magnon terms kept in the wave function; (b) $A_{\mathbf{k}}^{(n)}$ for different J_z/t.

In the Ising limit n_{mag} is identical to the average number of local spin deviations, $\langle \sum_i S_i^+ S_i^- \rangle = \langle \sum_i a_i^\dagger a_i \rangle$ and is proportional to the average string length l_{av} of flipped spins in the Néel state created by the motion of the hole. For $J/t \ll 1$ one may assume a linear string potential which implies $n_{mag} \propto l_{av} \propto (t/J)^{1/3}$. In Fig. 2 n_{mag} is shown as a function of J/t calculated with up to 40 magnon terms in the wave function. For $J/t \ll 1$ our result is in quantitative agreement with $n_{mag} = 1.4(t/J)^{1/3}$ calculated by Mattis and Chen.[16] In the opposite limit $J/t \gg 1$ only the leading term $m = 1$ in the wave function is relevant, therefore the asymptotic result is $n_{mag} \propto (t/J)^2$.

The spatial distribution of spin-deviations around the hole is given by the correlation function

$$N_{\mathbf{R}} = \langle \Psi_{\mathbf{k}\tau}^{(n)} | \sum_i n_i a_{i+\mathbf{R}}^\dagger a_{i+\mathbf{R}} | \Psi_{\mathbf{k}\tau}^{(n)} \rangle \equiv \langle n_0 (a_{\mathbf{R}}^\dagger a_{\mathbf{R}}) \rangle, \tag{22}$$

where $n_i = h_i^\dagger h_i$ is the density operator for holes. Fig. 3 shows the distribution of bosons around the hole, $N_{\mathbf{R}} = \langle n_0 (a_{\mathbf{R}}^\dagger a_{\mathbf{R}}) \rangle$, calculated in the Ising limit for $J_z/t = 0.002$ and 0.4. Within LSW approximation $\langle n_0 (a_{\mathbf{R}}^\dagger a_{\mathbf{R}}) \rangle$ is equivalent to $\langle n_0 (S_{\mathbf{R}}^+ S_{\mathbf{R}}^-) \rangle$. The correlation function $N_{\mathbf{R}}$ can therefore be used as a suitable definition of the *spin polaron* and consequently of its spatial size. For the spatial dependence we found $N_{\mathbf{R}} \propto \exp[-(R/R_s)^{3/2}]$. The size of the polaron can be characterized by a radius R_p which encloses a given fraction $p = \sum_{R<R_p} N_{\mathbf{R}}/n_{\text{mag}}$ of the polaron. For $p \geq 0.5$ and $J/t \geq 0.002$ we obtained the scaling $R_p \propto (t/J)^{1/6}$ with $R_{0.9} \sim 2$ for $J/t = 0.2$. The total number of bosons, and the scaling of the polaron size as well as its asymptotical R dependence are consistent with the picture of the random motion of the hole confined by a linear string potential. The average path length[17] scales as $l \propto n_{\text{tot}} \propto J^{-1/3}$ and as a consequence of the 2-dimensional random-walk of the hole the radius follows as $R_p \propto l^{1/2}$.

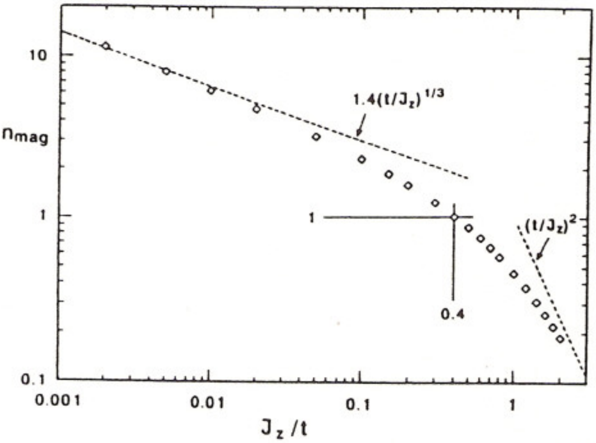

Fig. 2. Total number of spin-deviations contributing to the spin-polaron in the case of the t-J_z model

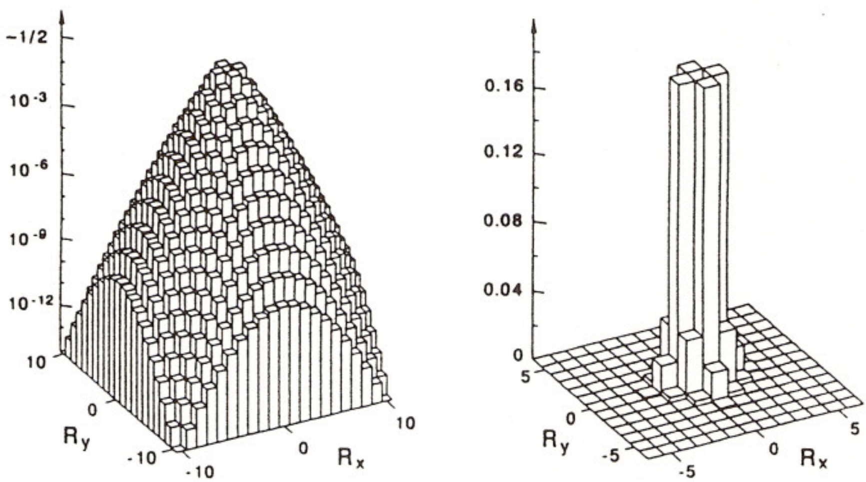

Fig. 3. Spatial distribution of spin deviations around the hole for the t-J_z model (a) $J_z = 0.002$ (log-scale) and (b) 0.4 (linear scale).

To conclude this Section we mention the approximations that have been made implicitely in the present treatment of the t-J_z model: (i) Comparing with the so called retraceable path approximation by Brinkman and Rice[2] our approach neglects the constraint that a hole can visit in a single step only $(z-1)$ neighbors and is not allowed to move back to the site from which it came. This constraint can also be incorporated and for a discussion concerning the Green's function we refer to Ref.[11] . (ii) As in the retraceable-path approximation processes are droped where holes perform loops. Such processes introduce a momentum dependence into the problem, but they are unimportant as long as J_z is not small.

While the approximation (i) is of quantitative importance for the $t-J_z$ model, e.g. the spectral weight in $ImG(\omega)$ extends over an ω-range of 8t instead of about 7t when this approximation is not made, the same approximation appears to be of minor importance in the $t-J$ model,[11] which we will discuss now.

4. Role of Quantum Fluctuations: The $t-J$ Model

The important new features of the $t-J$ model are (i) the spin-dynamics described by antiferromagnetic spin waves, which have linear dispersion around $q=(0,0)$ and (π,π), respectively. (ii) The ground state of the model in 2D is a quantum Néel state, i.e. more complex than the simple classical Néel ground state of the $t-J_z$ model. An immediate consequence of (i) is that a spin-deviation which is created by the hopping hole will move away from the hole in form of a spin-wave until it is reabsorbed at a later instance.

In Fig. 4a the norm $\mathcal{N}_k$ versus J/t for the $t-J$ model is shown for different number n of magnons kept in the wave function. For $J=0.4$ three magnon contributions in the wave function are required to fullfil the norm. In Fig. 4b $N_{\mathbf{R}}=\langle n_0(a^\dagger_{\mathbf{R}}a_{\mathbf{R}})\rangle - N_{\mathbf{AFM}}$ is shown for $J/t=0.4$ and $\mathbf{k}=(\pi/2,\pi/2)$. Here we have subtracted the large contribution $N_{AFM}=0.197$ from quantum fluctuations in the ground state in the absence of the hole. The shape of the polaron is extended in the direction of the QP momentum which reflects a quasi one-dimensional motion of the polaron. This is consistent with the asymmetry of the QP energy band in the "hole pocket", where the effective next-nearest neighbor hopping for the $(1,1)$ direction is $\sim 5\times$ that of the $(1,-1)$ direction.[10,11] The asymmetry is most pronounced at $\mathbf{k}=(\pi/2,\pi/2)$, and gradually vanishes away from the QP energy minimum and disappears at $k=0$ and $\mathbf{k}=(\pi,0)$.

Various more complicated spin-correlation functions were studied recently for the t-J model and we refer to the original reference [11]. All correlation functions show a pronounced spatial dependence which strongly depends on the momentum of the quasiparticle. All correlation functions were found to be in close agreement with results from diagonalization studies. Since the magnetic excitations $\omega_{\mathbf{q}}$ vanish linearly with $\mathbf{q}$, perturbations decay as power laws. For example $N_{\mathbf{R}}\sim R^{-2}$. Explicit results for other correlation function are given in Ref.[11].

It is the random motion of the hole on scale t which leads to the large increase of spin-fluctuations around the hole. This is the origin of the rapid disappearance of antiferromagnetic long-range order at quite small doping concentrations[18] and the strong spin-wave renormalization.[19,20] Apart from this rapid incoherent motion, the polaron as an entity propagates coherently with a dispersion of order J.

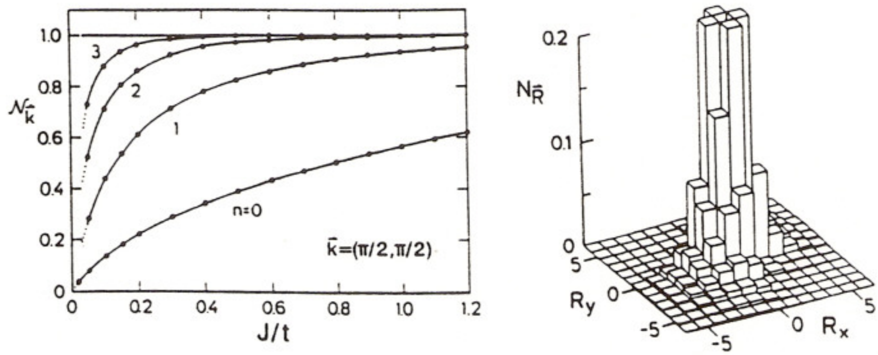

Fig. 4. (a) $\mathcal{N}_k$ versus J/t for the $t-J$ model and (b) Spatial distribution of spin deviations around the hole for $J = 0.4$ and $\mathbf{k} = (\pi/2, \pi/2)$.

5. Summary

We have derived the wave function of a quasiparticle in an antiferromagnet within selfconsistent Born approximation. Various correlation functions calculated from this wave function show that the scBA gives an accurate picture of the relaxation of the spin system around the hole.

Finally we would like to mention that electron-phonon coupling can be incorporated in this framework on the same footing as the coupling to spin-fluctuations.[21] Since the role of electron-phonon interactions in high-T_c superconductors is still a topic of debate, this feature will perhaps prove useful to shed light on the interplay between strong correlations and electron-phonon interactions.

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