Electron-momentum distribution function and spectral function in the t-J model

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The momentum distribution function and electron spectral function for mobile holes in an antiferromagnet as described by the t-J model are discussed. The calculations are done using a trial wave function for the coherent motion of an individual hole based on a string picture. To discuss finite concentrations, the rigid-band approximation is assumed to be valid. Despite this both quantities considered are qualitatively similar to what one would expect for weakly interacting particles occupying the tight-binding band calculated from the hopping term in the Hamiltonian.

I. INTRODUCTION

The problem of strongly interacting fermions on a lattice has received considerable attention in recent years. This is because one can hope to gain some insight into the nature of the carriers responsible for high temperature superconductivity. The simplest model Hamiltonian which incorporates the key features of the strong correlation limit is the t-J Hamiltonian:[1]

$$H_{t\text{-}J} = -t \sum_{\langle i,j\rangle,\sigma} (\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \text{H.c.}) + J \sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j \ . \tag{1}$$

Here the $\mathbf{S}_i$ are the electronic spin operators and the sum over $\langle i,j\rangle$ stands for a summation over all pairs of nearest neighbors on a two-dimensional square lattice. The operators $\hat{c}^{\dagger}_{i,\sigma}$ can be expressed in terms of ordinary fermion operators as $c^{\dagger}_{i,\sigma}(1-n_{i,-\sigma})$.

When the number of electrons is equal to the number of lattice sites the t-J model reduces to the Heisenberg antiferromagnet (HAF). This may be viewed as a system where the correlations dominate the physics completely. The momentum distribution function for electrons in the ground state of the HAF is constant throughout the Brillouin zone and there is no more reminiscence of the Fermi surface for the free electrons. On the other hand, when the number of electrons is much smaller than the number of sites one might expect the system to behave like a Fermi liquid with a discontinuity in the momentum distribution function consistent with Luttinger's theorem. Then one may ask in which way the system performs the "crossover" between this two limiting cases. Especially one might ask whether there is already some reminiscence of the Fermi liquid behavior near half filling, i.e., for a few holes in an antiferromagnet.

The problem of one single hole moving through a "background" of spins has been discussed in considerable detail.[2–5] It turns out that one can develop a rather simple and intuitive picture for this problem. It is well known that when a hole is created at some site j in a Néel-ordered spin state and allowed to hop around, it will feel some "effective potential" due to the formation of "strings."[6,7] This potential tends to localize the hole around the site j. Let us denote a state generated by ν-fold forward hopping starting from the Néel state with the electron at site j removed by $|j,\nu,\mathcal{P},\rangle$. The symbol $\mathcal{P}$ denotes a set of numbers which in some way parametrize the geometry of the path which the hole has taken. Then one can make the following ansatz for the (localized) ground state of $H_{t\text{-}J}$ in the subspace of string states with starting point j:

$$|\Phi_j\rangle = \sum_{\nu} \alpha_{\nu} \left(\sum_{\mathcal{P}} |j,\nu,\mathcal{P},\rangle \right) \ . \tag{2}$$

The inner sum in this expression runs over all different paths of length ν and the coefficients α_{ν} are to be determined from the requirement of minimum total energy. It is advantageous to choose the energy of the Néel state with one electron removed as the zero of energy and to make the following approximation:

$$H_{I\text{sing}}|j,\nu,\mathcal{P},\rangle = \frac{J}{2}[(z-2)\nu + 1 - \delta_{\nu,0}]|j,\nu,\mathcal{P}\rangle \ , \tag{3}$$

where z is the number of nearest neighbors (i.e., z=4). Then one can introduce a new function β_{ν} by $\beta_{\nu} = (z-1)^{\nu/2}\alpha_{\nu}$ and show that the β's can be determined from the discrete version of a one-dimensional Schrödinger equation with a linearly ascending potential.[6,7] From the numerical solution of this one can see that the α's are a rapidly decreasing function of the path length ν.

The t-J Hamiltonian now allows for a number of processes by which the hole can escape from the string potential. The most important one is the truncation of the string by the transverse part of the Heisenberg exchange, another less important process is hopping along a spiral path as first discussed by Brinkman and Rice.[8,4] With each of these processes one can associate some sort of potential barrier which the hole has to penetrate. This is because in each of these processes the number of frustrated bonds first increases and then decreases again. Thus one can see an effective tight-binding Hamiltonian emerge: while moving through the lattice the hole mostly finds itself in localized states like $|\Phi_j\rangle$ where it is bound to one particular site by the string potential and by means of the various processes mentioned above it can tunnel from

one of these localized states to the next one. It turns out that these tunneling processes connect only the sites of one sublattice, so the most natural ansatz for the wave function of the hole is simply

$$|\Psi(\mathbf{k})\rangle = \left(\frac{2}{N}\right)^{1/2} \sum_j e^{-i\mathbf{k}\cdot\mathbf{R}_j} |\Phi_j\rangle \ . \tag{4}$$

Here N denotes the number of sites in the system and the summation over j runs over the sites of one sublattice only. The dispersion relation $E(\mathbf{k})$ for coherent motion can be obtained by forming the expectation value of the full t-J Hamiltonian with the wave function (4). It turns out[9,10] that this simple formalism can reproduce the results of finite-size diagonalizations[11-13] and other numerical methods[4,5,14] with remarkable accuracy.

If one wants to extend this theory to a finite concentration of holes the first guess would be to assume that the "quasiparticles" may be treated as weakly interacting fermions and to fill up the calculated band ("rigid-band approximation"). This can be made plausible by the following consideration: any string state $|j,\nu,\mathcal{P},\rangle$ can be written as a product of a number of spin raising and lowering operators and precisely one annihilation operator acting on the Néel state:

$$\begin{aligned} |j,\nu,\mathcal{P},\rangle &= (-1)^\nu \prod_\lambda S^+_{i_\lambda} \prod_\mu S^-_{i_\mu} \hat{c}_{l,\sigma(l)} |\Phi_{\text{Néel}}\rangle \\ &= \tilde{c}_{j,\mathcal{P},\nu} |\Phi_{\text{Néel}}\rangle \ , \end{aligned} \tag{5}$$

where the sites i_λ, i_μ, l are determined by the geometry of the string and the second equation is the definition of the "string creation operator" $\tilde{c}_{j,\mathcal{P},\nu}$. Using this definition one can introduce

$$\begin{aligned} \tilde{c}_j &= \sum_\nu \alpha_\nu \left(\sum_{\mathcal{P}} \tilde{c}_{j,\mathcal{P},\nu} \right) \ , \\ \tilde{c}_{\mathbf{k}} &= \left(\frac{2}{N}\right)^{1/2} \sum_j e^{-i\mathbf{k}\cdot\mathbf{R}_j} \tilde{c}_j \ , \\ |\Psi(\mathbf{k})\rangle &= \tilde{c}_{\mathbf{k}} |\Phi_{\text{Néel}}\rangle \ . \end{aligned} \tag{6}$$

Next one can see that the anticommutation relations of the "string creation operators" (5) are determined entirely by their "core" fermion operators $\hat{c}_{l,\sigma}$ provided the two strings do not cross. One can conclude that any two of the operators $\tilde{c}_j$, $\tilde{c}_{j'}$ will anticommute provided the distance between the sites j, j' is larger than the "diameter" of the localized states (2), i.e., a few lattice spacings. Thus one can conclude that the operators $\tilde{c}_{\mathbf{k}}$ obey fermion anticommutation relations to a good approximation. The deviations from simple anticommutation relations for these operators are due to the overlap of the two "clouds of spin defects" which the two holes carry with them. They may be described in terms of effective interaction terms in the "quasiparticle Hamiltonian."[15] When this interaction is neglected as a simplest approximation one might indeed expect that the band evaluated from the ansatz (4) is simply filled up for a not too large number of holes. Then one would get four hole pockets around the four degenerate minima of the tight-binding dispersion relation which are located at $(\pm\pi/2, \pm\pi/2)$. Also it is quite plausible that similar considerations might be applied to the motion of holes in any translationally invariant "spin background" which has strong short-range antiferromagnetic correlations ("spin liquid"). The problem is that this naive "quasiparticle Fermi surface" has not been observed in photoemission experiments on real high temperature superconductors.[16] Rather these experiments seem to show a Fermi surface which is roughly consistent with LDA band-structure calculations, i.e., a simple "Fermi liquid picture." In addition, exact diagonalization studies[17] of the t-J model on small clusters show that the momentum distribution function for electrons at a hole concentration of 10% (two holes in a 20-site cluster) is similar to what one would expect from the Luttinger theorem for weakly interacting Fermions occupying the simple nearest-neighbor hopping tight-binding band: the momentum distribution function is large inside the Fermi surface evaluated from the tight-binding band with the given electron number and small outside. Especially the maximum of the occupation number is in the center of the Brillouin zone and the minimum at the corner. The same overall behavior of the momentum distribution function has also been found in a numerical study of the Hubbard model.[18] It is virtually impossible to understand this in the framework of the theory for quasiparticles outlined above since there the center and the corner of the Brillouin zone are actually identical due to the sublattice structure.

In the following some arguments will be presented indicating that the discrepancy between the "string picture" and the "Fermi liquid picture" is actually not as severe as it might seem. To see this one simply has to take into account the many-body structure of the wave function (4) which prevents naive application of concepts from one-particle physics.

II. ELECTRON MOMENTUM DISTRIBUTION

Let us first turn to the evaluation of the momentum distribution function for the case of one single hole. In other words the expectation value of the operator

$$n_{\mathbf{k},\sigma} = c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} \tag{7}$$

with the ground-state wave function for $N/2$ spin-down electrons and $N/2-1$ spin-up electrons has to be evaluated. Here some care is necessary. The wave function (4) was constructed from the Néel state, i.e., a state with explicitly broken symmetry. If one wants to compare this with the results of exact diagonalizations this should be avoided since there is no broken symmetry in a finite system. Therefore as the ground state with one hole one might choose the following state:

$$|\Psi_0\rangle = \frac{1}{\sqrt{2}} \left(|\Psi(\mathbf{k}_0)\rangle + |\tilde{\Psi}(\mathbf{k}_0)\rangle \right) \ . \tag{8}$$

Here $|\Psi(\mathbf{k}_0)\rangle$ is a state of the type (4) which was constructed starting from a Néel state where the spin at the origin of the coordinate system is up whereas the initial state for the construction of $|\tilde{\Psi}(\mathbf{k}_0)\rangle$ is just the time re-

versed Néel state. In both states the hole is supposed to sit on the ↑ sublattice so that the total z spin of $|\Psi_0\rangle$ is $-\frac{1}{2}$. The relative sign between the two states in (8) is fixed if one requires this state to have total momentum $\mathbf{k}_0$. If one neglects off-diagonal matrix elements like $\langle\Psi(\mathbf{k}_0)|n_{\mathbf{k},\sigma}|\tilde{\Psi}(\mathbf{k}_0)\rangle$ (as will be done in the following calculations) the relative phase of the two states in expression (8) is actually arbitrary. This procedure might also be appropriate to "simulate" a system where there is no more long-range order in the spin background but still strong short-range antiferromagnetic correlations.

Using the definition

$$c_{\mathbf{k},\sigma} = \frac{1}{\sqrt{N}} \sum_j e^{-i\mathbf{k}\cdot\mathbf{R}_j} c_{j,\sigma} \tag{9}$$

and (4) one can show that the expectation value of this operator in the state $|\Psi_0\rangle$ can be written as

$$\langle\Psi_0|n_{\mathbf{k},\sigma}|\Psi_0\rangle = \sum_l e^{-i\mathbf{k}\cdot\mathbf{R}_l} \langle\Psi_0|c^\dagger_{0,\sigma} c_{l,\sigma}|\Psi_0\rangle \ . \tag{10}$$

Next one can see that

$$\sum_l e^{-i\mathbf{k}\cdot\mathbf{R}_l} \langle\Psi(\mathbf{k}_0)|c^\dagger_{0,\sigma} c_{l,\sigma}|\Psi(\mathbf{k}_0)\rangle$$

$$= \frac{2}{N} \sum_{j,j',l} e^{-i[\mathbf{k}_0\cdot(\mathbf{R}_j - \mathbf{R}_{j'}) + \mathbf{k}\cdot\mathbf{R}_l]} \langle\Phi_{j'}|c^\dagger_{0,\sigma} c_{l,\sigma}|\Phi_j\rangle \ . \tag{11}$$

Thereby the summation over j, j' is restricted to the ↑ sublattice whereas the summation over l includes all sites. The task is now to figure out all triples of sites j, j', l for which the matrix element $\langle\Phi_{j'}|c^\dagger_{0,\sigma} c_{l,\sigma}|\Phi_j\rangle$ is different from zero.

One can always choose l=0 and $j = j'$. As can be seen from (11) there remains no dependence on either $\mathbf{k}_0$ or $\mathbf{k}$, in other words the corresponding contribution to the momentum distribution is simply a constant in the Brillouin zone. This constant is somewhat reduced as compared to the value for the HAF. For example, if j is a second-nearest neighbor of 0 one can verify that

$$\langle\Phi_j|c^\dagger_{0,\uparrow} c_{0,\uparrow}|\Phi_j\rangle = 1 - 2\sum_{\nu=2}^{\infty} (z-1)^{\nu-2} \alpha_\nu^2 + \cdots \ . \tag{12}$$

Namely, 0 is a site on the up sublattice and therefore the expectation value on the left is always different from zero provided the hole is not sitting at the site 0 or has run over this site. The probability for these last two possibilities is just given by the subtracted terms on the right-hand side. Thereby it is assumed that the hole has reached the site 0 by the shortest way possible, i.e., by two hops. There will be corrections but these can be seen to be proportional to α's with rather high indices, so they can be neglected. In a completely analogous way one can discuss the case where j is a third-nearest neighbor of 0 and so on. Eventually one gets the following contributions from the triples with $l = 0, j = j'$:

$$\delta\langle\Psi_0|n_{\mathbf{k},\uparrow}|\Psi_0\rangle = \frac{1}{2} - \frac{1}{N}\left(1 + \frac{12}{(z-1)^2}\sum_{\nu=2}^{\infty}\beta_\nu^2\right) \ ,$$

$$\delta\langle\Psi_0|n_{\mathbf{k},\downarrow}|\Psi_0\rangle = \frac{1}{N}\left(\frac{4}{z-1}\sum_{\nu=1}^{\infty}\beta_\nu^2 + \cdots\right) \ , \tag{13}$$

and if one replaces $|\Psi(\mathbf{k}_0)\rangle \to |\tilde{\Psi}(\mathbf{k}_0)\rangle$ in (11) one obtains additional contributions of

$$\delta\langle\Psi_0|n_{\mathbf{k},\uparrow}|\Psi_0\rangle = \frac{1}{N}\frac{4}{z-1}\sum_{\nu=2}^{\infty}\beta_\nu^2 \ ,$$

$$\delta\langle\Psi_0|n_{\mathbf{k},\downarrow}|\Psi_0\rangle = \frac{1}{2} - \frac{1}{N}\left(\frac{4}{z-1}\sum_{\nu=1}^{\infty}\beta_\nu^2 + \cdots\right) \ . \tag{14}$$

Thereby some corrections which are proportional to α's with high indices have been omitted. So far the momentum distribution function is simply constant throughout the Brillouin zone.

A second possibility to obtain a nonvanishing matrix element in (11) is to choose $j = 0$ and $j' = l$. It is easy to show that

$$\langle\Phi_l|c_{l,\uparrow} c^\dagger_{0,\uparrow}|\Phi_0\rangle = \alpha_0^2 \ , \tag{15}$$

so that one obtains the following contribution to $\langle n_{\mathbf{k},\uparrow}\rangle$:

$$\delta\langle\Psi_0|n_{\mathbf{k},\uparrow}|\Psi_0\rangle = -\frac{1}{2}\alpha_0^2\left(\delta_{\mathbf{k},\mathbf{k}_0} + \delta_{\mathbf{k},\mathbf{k}_0+\mathbf{K}} - \frac{2}{N}\right) \ , \tag{16}$$

where $\mathbf{K} = (\pi, \pi)$. Within the framework of the rigid-band approximation the contributions considered so far would give a momentum distribution function which is similar to what one naively would expect from the "hole pocket" picture: the momentum distribution function is piecewise constant in the Brillouin zone and it is larger outside the hole pockets than inside. Note however that the discontinuity at the surface of the pockets is much smaller than one would expect it if one would assume that the quasiparticles were simply "holes." This can be seen from Fig. 1 where the quantity $\Delta = \alpha_0^2/2$ which de-

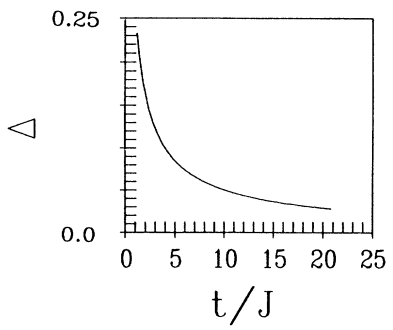

FIG. 1. The magnitude of the discontinuity at the surface of the hole pockets Δ as a function of the ratio t/J.

TABLE I. Various contributions to the momentum distribution function for up-spin electrons. For each type of process only one "typical" triple of sites l, j, j' is listed.

$\mathbf{R}_l$	$\mathbf{R}_j$	$\mathbf{R}_{j'}$	$N\delta\langle\Psi_0\vert n_{\mathbf{k},\uparrow}\vert\Psi_0\rangle$
(1,1)	(0,2)	(0,2)	$-4\alpha_2^2 4\cos(k_x)\cos(k_y)$
(2,0)	(1,1)	(1,1)	$-2\alpha_2^2[2\cos(2k_x)+2\cos(2k_y)]$
(1,0)	(4,0)	(4,0)	$21\alpha_3\alpha_4[2\cos(k_x)+2\cos(k_y)]$
(1,1)	(0,4)	(0,4)	$-28\alpha_4^2 4\cos(k_x)\cos(k_y)$
(2,0)	(1,3)	(1,3)	$-14\alpha_4^2[2\cos(2k_x)+2\cos(2k_y)]$

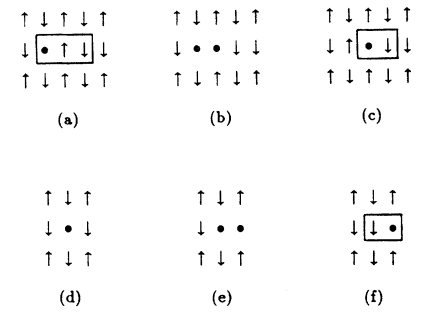

FIG. 2. Two processes which contribute to the momentum distribution function.

termines this discontinuity is shown as a function of t/J. It is interesting to note that the behavior of the discontinuity is in qualitative agreement to what one would expect from the large-U Hubbard model. Since $t/J \sim U/t$ one would expect that for increasing t/J the discontinuity becomes smaller which is indeed the case. It should be mentioned that from (14) and (16) one can readily see that the sum of $\langle n_{\mathbf{k},\sigma}\rangle$ over all $\mathbf{k}$ is indeed equal to the number of electrons with the respective spin in the system.

Next one can see that there are also additional contributions to the momentum distribution function which change this picture. To that end let us consider the case $l \neq 0$. For example, if l is a nearest neighbor of 0 the process shown in Figs. 2(a)–2(c) becomes possible. The state shown in Fig. 2(a) is a string state created by two hops. Thus it has expansion coefficient α_2 in its localized state $|\Phi_j\rangle$ (j is the starting point of the string). By annihilating an up-spin electron the state shown in Fig. 2(b) can be obtained. Creation of an up-spin electron leads to the state shown in Fig. 2(c) which has expansion coefficient α_1 in the state $|\Phi_j\rangle$. Here one has $j = j'$ and the phase factor associated with this contribution is e^{-ik_x}. Taking into account all the equivalent processes one obtains the following contribution:

$$\delta\langle\Psi_0|n_{\mathbf{k},\uparrow}|\Psi_0\rangle = \frac{1}{N}3\alpha_1\alpha_2[2\cos(k_x)+2\cos(k_y)] \ . \qquad (17)$$

The additional factor of 3 is due to the fact that for fixed l there are actually three different choices of $j = j'$ such that the process described above is possible. There are two points which should be noted: first of all the expression is independent of the ground-state momentum $\mathbf{k}_0$. This means that at finite concentration c of spin-up holes in this expression one should replace $1/N \rightarrow c$. Secondly, this expression removes the symmetry between $\mathbf{k} = (0,0)$ and $\mathbf{k} = (\pi,\pi)$. This contribution makes sure, that the momentum distribution function is larger in the center of the Brillouin zone than at the corner, i.e., the momentum distribution function does not resemble the reduction of the Brillouin zone due to the sublattice structure of the Néel state. This at first sight a paradoxical result can be understood if one takes into account that the "real hole" does not see the sublattice structure in the Néel state as long as it is hopping "inside" of states like $|\Phi_j\rangle$. As can be seen from the derivation of (17) this contribution is determined entirely by the "internal structure" of the wave function $|\Phi_j\rangle$. Next one can consider the process shown in Fig. 2(d)–2(f). The state shown in Fig. 2(d) is a "string of length zero." The expansion coefficient of this state is α_0 in its state $|\Phi_j\rangle$. When a spin-up electron is annihilated the state shown in Fig. 2(e) can be obtained. The subsequent creation of a spin-down electron leads to the state shown in Fig. 2(f) which has expansion coefficient α_1 in the state $|\Phi_j\rangle$. In this process one has $j = j' = 0$ and the phase factor associated with this contribution is e^{ik_x}. By summing the contributions from all equivalent processes one obtains

$$\delta\langle\Psi_0|n_{\mathbf{k},\downarrow}|\Psi_0\rangle = \frac{1}{N}\alpha_0\alpha_1[2\cos(k_x)+2\cos(k_y)] \ . \qquad (18)$$

There are quite a lot of additional triples which give nonvanishing contributions to (11). The calculation of the individual contributions proceeds in the same way as shown above. Therefore only the most important contributions are listed in Tables I and II. The expressions for triples which are not listed in these tables can be shown

TABLE II. Various contributions to the momentum distribution function for down-spin electrons. For each type of process only one "typical" triple of sites l, j, j' is listed.

$\mathbf{R}_l$	$\mathbf{R}_j$	$\mathbf{R}'_j$	$N\delta\langle\Psi_0\vert n_{\mathbf{k},\downarrow}\vert\Psi_0\rangle$
(1,1)	(1,1)	(0,0)	$-2\alpha_2^2 4\cos(k_{0,x}+k_x)\cos(k_{0,y}+k_y)$
(2,0)	(2,0)	(0,0)	$-4\alpha_2^2\{2\cos[2(k_{0,x}+k_x)]+2\cos[2(k_{0,y}+k_y)]\}$
(1,0)	(0,2)	(0,2)	$9\alpha_2\alpha_3[2\cos(k_x)+2\cos(k_y)]$
(1,1)	(1,1)	(0,0)	$-4\alpha_4^2 4\cos(k_{0,x}+k_x)\cos(k_{0,y}+k_y)$
(2,0)	(2,0)	(0,0)	$-6\alpha_4^2\{2\cos[2(k_{0,x}+k_x)]+2\cos[2(k_{0,y}+k_y)]\}$

TABLE III. Various contributions to the momentum distribution function for up-spin electrons as obtained by replacing $|\Psi(\mathbf{k}_0)\rangle \rightarrow |\tilde{\Psi}(\mathbf{k}_0)\rangle$ in (11). For each type of process only one "typical" triple of sites l, j, j' is listed.

$\mathbf{R}_l$	$\mathbf{R}_j$	$\mathbf{R}_{j'}$	$N\delta\langle\Psi_0\|n_{\mathbf{k},\uparrow}\|\Psi_0\rangle$
(1,0)	(−1,0)	(−1,0)	$3\alpha_1\alpha_2[2\cos(k_x)+2\cos(k_y)]$
(1,1)	(1,0)	(0,1)	$-4\alpha_3^2[\cos(k_{0,x}-k_{0,y})\cos(k_x+k_y)+\cos(k_{0,x}+k_{0,y})\cos(k_x-k_y)]$
(1,0)	(−3,0)	(−3,0)	$21\alpha_3\alpha_4[2\cos(k_x)+2\cos(k_y)]$

to be proportional to products of α's with rather high indices and due to the rapid decay of this function they are small. Even the terms proportional to say α_4^2 give a very small contribution despite the large combinatoric prefactors which multiply them.

In a completely analogous fashion one can also evaluate the different contributions to the expectation value of $n_{\mathbf{k},\sigma}$ obtained by replacing $|\Psi(\mathbf{k}_0)\rangle \rightarrow |\tilde{\Psi}(\mathbf{k}_0)\rangle$ in (11). They are listed in Tables III and IV. Summing up all the different contributions one finally obtains the total momentum distribution function. This function is shown in Fig. 3 for a hole concentration of 15%. One can see that the hole pockets are superimposed over a function which is similar to a "smeared out" version of the momentum distribution function as one would expect it for free particles occupying the noninteracting band structure.

Another way to exemplify the results of the calculation is to "simulate" a finite-size diagonalization by taking N equal to the number of sites in the finite cluster and setting $\mathbf{k}_0$ equal to the momentum of the ground state of the cluster. As an example for such a calculation in Table V the momentum distribution function as obtained from the above theory is shown for some allowed $\mathbf{k}$ points in an 18-site cluster [the ground-state momentum is equal to $(-2\pi/3, 0)$[11]]. Again one can recognize that superimposed over the "pocket" at the position of the ground-state momentum there is the contribution due to the "internal structure" of the quasiparticles which produces a larger value of the momentum distribution function inside the antiferromagnetic Brillouin zone than outside. The values obtained in this way are in reasonable agreement with the data from an actual finite-size diagonalization.[21]

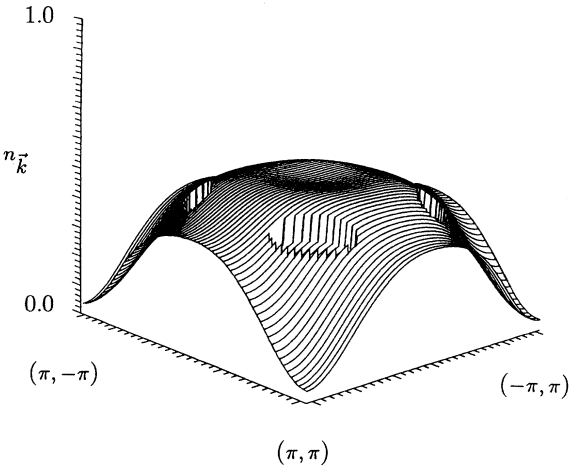

FIG. 3. Momentum distribution function in the Brillouin zone for a hole concentration of 15% as obtained within the rigid-band approximation. The ratio $t/J = 5$. The Fermi energy as well as the position of the pockets has been calculated from the one-particle dispersion relation.

It is rather difficult to make a quantitative comparison with exact diagonalizations for two holes in a finite cluster.[17] There one usually obtains a binding energy of $\sim J$ indicating a strong interaction of the two holes. One may conclude that the ground state for two holes should be a superposition of states where the total momentum is distributed over the two holes in all possible ways. Thus there is no well-defined momentum $\mathbf{k}_0$ which would determine the position of the hole pockets. Thus it is not astonishing to see that in an exact diagonalization with two holes[17] there are virtually no more hole pockets: they are probably smeared out due to the strong interaction of the two holes.

From the preceding results one can extract the following scenario for the change of the momentum distribution function with increasing hole density: At a low concentration of holes one should have well-defined pockets and the difference in the momentum distribution function between the center and the corner of the Brillouin zone is small. As more and more holes are added, the area covered by the pockets will grow and the difference between the center and the corner of the Brillouin zone will grow linearly with the concentration of holes. As the spins become more and more diluted however one may expect that the short-range antiferromagnetic spin correlations be less pronounced. Thus one might argue that the "string potential" will become flatter [i.e., in Eq. (3) one should introduce an "effective J" which is smaller

TABLE IV. Various contributions to the momentum distribution function for down-spin electrons as obtained by replacing $|\Psi(\mathbf{k}_0)\rangle \rightarrow |\tilde{\Psi}(\mathbf{k}_0)\rangle$ in (11). For each type of process only one "typical" triple of sites l, j, j' is listed.

$\mathbf{R}_l$	$\mathbf{R}_j$	$\mathbf{R}_{j'}$	$N\delta\langle\Psi_0\|n_{\mathbf{k},\downarrow}\|\Psi_0\rangle$
(1,0)	(1,0)	(1,0)	$\alpha_0\alpha_1[2\cos(k_x)+2\cos(k_y)]$
(1,1)	(1,0)	(1,0)	$-2\alpha_1^2 4\cos(k_x)\cos(k_y)$
(2,0)	(1,0)	(1,0)	$-\alpha_1^2[2\cos(2k_x)+2\cos(2k_y)]$
(1,0)	(3,0)	(3,0)	$9\alpha_2\alpha_3[2\cos(k_x)+2\cos(k_y)]$
(1,1)	(3,0)	(3,0)	$-12\alpha_3^2 4\cos(k_x)\cos(k_y)$
(2,0)	(2,1)	(2,1)	$-6\alpha_3^2[2\cos(2k_x)+2\cos(2k_y)]$

TABLE V. Momentum distribution in the ground state of an 18-site cluster with 9 spin-down electrons and 8 spin-up electrons as obtained from the variational ansatz. Thereby $t/J = 2.5$ and the momentum of the ground state $\mathbf{k}_0 = (-2\pi/3, 0)$.

k_x	k_y	$n_{\mathbf{k},\uparrow}$	$n_{\mathbf{k},\downarrow}$
0	0	0.4956	0.5278
$\frac{\pi}{3}$	$\frac{\pi}{3}$	0.4899	0.5498
$\frac{2\pi}{3}$	0	0.4804	0.5314
$-\frac{2\pi}{3}$	0	0.3395	0.5465
π	$\frac{\pi}{3}$	0.4491	0.5038
$\frac{\pi}{3}$	π	0.3367	0.4938
$\frac{2\pi}{3}$	$\frac{2\pi}{3}$	0.4273	0.4533
π	π	0.3704	0.3289

than the original one] and the wave functions (2) will be more delocalized. As can be seen from Fig. 1 the magnitude of the discontinuity in the momentum distribution function at the surface of the pockets would then decrease and the pockets would "fade away." On the other hand products like $\alpha_1\alpha_2$ which determine the magnitude of the difference in $n_{\mathbf{k}}$ between $\mathbf{k} = (0,0)$ and $\mathbf{k} = (\pi,\pi)$ would grow (at least initially) making the growth of the difference between center and corner stronger than linear with the hole concentration. Of course when the string potential is very flat the contributions proportional to α's with higher indices which have been neglected previously become appreciable and the simple theory outlined above will break down. All in all one may say that there is some reminiscence of the weak correlation limit already close to half filling. Thus the discrepancy between the low concentration limit with well-defined hole pockets and the high concentration limit with a Fermi surface consistent with the Luttinger theorem as observed in numerical studies on the t-J model[21] and the Hubbard model[18] is not as large as it might seem. Especially one might speculate about the possibility of a smooth transition between the high and low concentration regimes.

III. SPECTRAL FUNCTION

Let us now turn to the evaluation of the spectral function for the creation of a hole in the undoped system, i.e., the Heisenberg antiferromagnet (HAF). This is defined as

$$A(\mathbf{k},\omega) = -\frac{1}{\pi}\mathrm{Im}\langle\Psi_0|\hat{c}^{\dagger}_{\mathbf{k},\sigma}\frac{1}{\omega + E_0 - H_{t\text{-}J} + i0^+}\hat{c}_{\mathbf{k},\sigma}|\Psi_0\rangle \ . \tag{19}$$

Here $|\Psi_0\rangle$, E_0 denote the ground-state wave function and energy of the HAF. If one wants to calculate the contribution to this correlation function from the quasiparticle band one should replace

$$\frac{1}{\omega + E_0 - H_{t\text{-}J} + i0^+} \rightarrow \sum_{\mathbf{k}}\frac{|\Psi_\sigma(\mathbf{k})\rangle\langle\Psi_\sigma(\mathbf{k})|}{\omega + E_0 - E_B - E(\mathbf{k}) + i0^+} \ , \tag{20}$$

where the energy E_B is the "binding energy" of the states $|\Phi_j\rangle$ which can be determined numerically from the Schrödinger equation for the coefficients α_ν. The wave functions $|\Psi_\sigma(\mathbf{k})\rangle$ are defined in an analogous way as in (8):

$$|\Psi_\sigma(\mathbf{k})\rangle = \frac{1}{\sqrt{2}}(|\Psi(\mathbf{k})\rangle + |\tilde{\Psi}(\mathbf{k})\rangle) \ , \tag{21}$$

where the total z spin of the state is $-\sigma$ (i.e., the hole is sitting on the σ sublattice). This procedure is again necessary to compare with exact diagonalizations where broken symmetry does not occur. The dispersion of the quasiparticle pole is then given by the energy dispersion $E(\mathbf{k})$ and it has been shown that the numerical results are reproduced quite accurately by the variational ansatz.[9,10] Let us now try to evaluate the residuum of the quasiparticle peak. This is given by

$$r(\mathbf{k}) = |\langle\Psi_\sigma(\mathbf{k})|\hat{c}_{\mathbf{k},\sigma}|\Psi_0\rangle|^2 \ . \tag{22}$$

As a first approximation one may replace the ground state of the HAF by the superposition of two Néel states with opposite staggered magnetization. Thereby the coefficients of the two Néel states have to be equal in order to obtain a state with total momentum zero. Then one can see that

$$\langle\Psi_\sigma(\mathbf{k})|\hat{c}_{\mathbf{k},\sigma}|\Psi_0\rangle = \frac{1}{\sqrt{2}}\alpha_0 \ , \tag{23}$$

because any string state where the length of the string is greater than zero is orthogonal to the state obtained by taking out one spin from a Néel state. In order to find corrections to (23) one has to take into account the spin fluctuations in the ground state of the HAF. One may use, for example, a wave function proposed by Bartkowski[19] to describe the spin fluctuations. This reads

$$|\Phi_B\rangle = \prod_{n,\delta}(1 + \lambda_0 S^-_n S^+_{n+\delta})|\Phi_{\text{Néel}}\rangle \ . \tag{24}$$

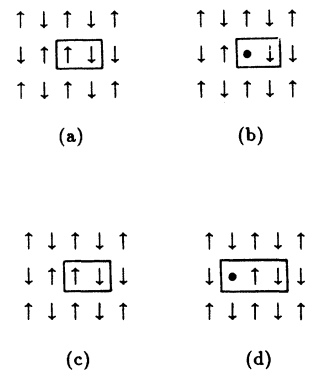

FIG. 4. Two processes contributing to the $\mathbf{k}$ dependence of the residuum of the hole Green's function.

The index n runs over all the sites of the "up sublattice," δ denotes the nearest neighbors, and λ_0 is a variational parameter. In the original paper by Bartkowski[19] it was found that $\lambda_0 \sim -0.17$. To avoid explicit symmetry breaking one should again use a superposition of two such functions which have been constructed starting from Néel states with opposite staggered magnetization. When spin fluctuations are present processes like the ones shown in Fig. 4 become possible. In the state shown in Fig. 4(a) there is a spin fluctuation present. Thus it is possible to annihilate an up-spin electron at a site where it would not have been possible in the Néel state. The resulting state [shown in Fig. 4(b)] is a "string state" where the length of the string is 1. Thus it has the expansion coefficient α_1 in its state $|\Phi_j\rangle$. Since the site j and the site, where the hole has been created, are nearest neighbors one obtains a phase factor of e^{ik_x}. Using similar procedures as in Ref. 10 one can show that the contribution to $r(\mathbf{k})$ from the process shown in Figs. 4(a) and 4(b) is approximately given by

$$\delta\langle\Psi_\sigma(\mathbf{k})|\hat{c}_{\mathbf{k},\sigma}|\Psi_0\rangle = -\frac{1}{\sqrt{2}}\lambda_0\alpha_1[2\cos(k_x)+2\cos(k_y)] . \tag{25}$$

In the state shown in Fig. 4(c) there is again a spin fluctuation present. When the spin-up electron on an adjacent site is annihilated a state like the one shown in Fig. 4(d) is obtained, which corresponds to a string of length 2 and therefore has the expansion coefficient α_2 in its state $|\Phi_j\rangle$. Summing over all equivalent processes one obtains a contribution of approximately

$$\delta\langle\Psi_\sigma(\mathbf{k})|\hat{c}_{\mathbf{k},\sigma}|\Psi_0\rangle = \frac{1}{\sqrt{2}}\lambda_0\alpha_2\,[\,8\cos(k_x)\cos(k_y) + 2\cos(2k_x) + 2\cos(2k_y)] . \tag{26}$$

Adding up the contributions (23), (25), (26), and squaring the sum one obtains the $\mathbf{k}$ dependence of the pole strength. A first check of this expression is possible by examining the dependence on the ratio t/J. Namely, Stephan *et al.*[20] have extracted the following dependence of the pole strength on the ratio t/J from their exact diagonalization results:

$$r = 0.3\left(\frac{J}{t}\right)^{0.6}, \quad \mathbf{k} = \left(0, \frac{2\pi}{3}\right) ,$$
$$r = 0.3\left(\frac{J}{t}\right)^{0.7}, \quad \mathbf{k} = \left(\frac{\pi}{3}, \frac{\pi}{3}\right) . \tag{27}$$

In Fig. 5 the ratio of these expressions and the calculated pole strength is shown as a function of t/J. One can see that it is close to unity more or less independently of t/J. Note that this is quite remarkable because the numerator and denominator change by a factor of $10^{0.7} \sim 5$ each. Thus the present theory gives a simple explanation for the scaling laws (27): since the slope of the string potential is proportional to J/t the function α_ν will be more and more sharply peaked at $\nu = 0$ as the ratio J/t increases. Since by annihilating an electron in the ground state of the HAF one creates predominantly short strings the pole strength must increase with J/t.

In Fig. 6 the dependence of the pole strength on the wave vector $\mathbf{k}$ is shown along some directions in the Brillouin zone and compared to data from an exact diagonalization.[11] Note the excellent agreement between our simple theory (which does not contain any adjustable parameter) and the numerical result. Another notable feature is, that this dependence on the wave vector is qualitatively similar to what one would expect from the "Fermi liquid picture": inside the Fermi surface as one would obtain it for a half-filled band of noninteracting electrons the residuum found here for the quasiparticles is small and it increases as one approaches the Fermi surface. This corresponds to the fact that in a Fermi liquid one would expect well-defined quasiparticles (i.e., an appreciable pole strength) only in the neighborhood of the Fermi surface. Outside the Fermi surface for noninteracting electrons the residuum decreases almost down to zero which means, for example, that in a photoemission experiment the corner of the Brillouin zone would appear to be unoccupied by electrons. This is in sharp contrast to what one would expect from the one-hole dispersion relation $E(\mathbf{k})$ because there the edge of the Brillouin zone is one of the maxima of the energy (i.e., it should be definitely unoccupied by holes, i.e., occupied by electrons).

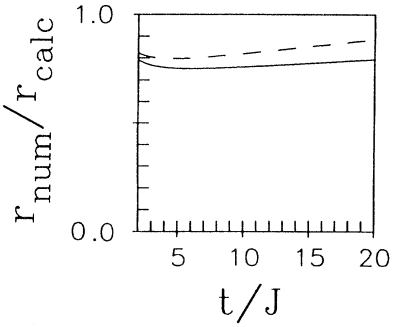

FIG. 5. Ratio of the calculated strength of the quasiparticle pole r_{calc} and the result obtained by Stephan *et al.* (Ref. 20). r_{num} as a function of t/J for $\mathbf{k} = (\pi/3, \pi/3)$ (solid line) and $\mathbf{k} = (0, 2\pi/3)$ (dashed line).

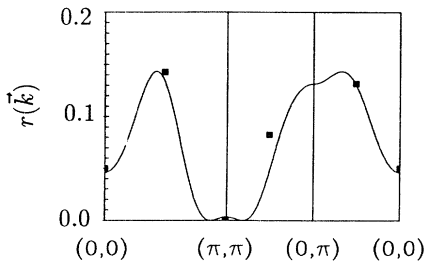

FIG. 6. Dependence of the strength of the quasiparticle pole on the wave vector $\mathbf{k}$ along some directions in the Brillouin zone. The ratio t/J is equal to 2.5. The squares are results from an exact diagonalization of a 4×4 cluster (Ref. 11).

Next consider a finite concentration of holes and let us assume that the rigid-band approximation is valid. Then for $\mathbf{k}$ points inside the hole pockets the pole strength should be equal to zero whereas it should be unchanged for the other ones. Thus one will again have the "pockets" superimposed over a $\mathbf{k}$ dependent part which has some similarity to a "washed-out" version of the Fermi liquid behavior.

An alternative way to obtain the momentum distribution function would be to integrate the spectral function (19) over all frequencies from the Fermi energy to infinity. While this cannot be done within the framework of the present variational ansatz it is easy to see that the value for the magnitude of the discontinuity in the momentum distribution function at the surface of the pockets obtained in this way is consistent with the previous calculation if only the contribution (23) is kept in the calculation of the pole strength. This is quite clear, because in the calculation of the momentum distribution function spin fluctuations were neglected completely. This is quite reasonable since the most important correction (25) vanishes at the surface of the magnetic Brillouin zone, i.e., in the region of $\mathbf{k}$ space where the pockets are located. However one can see that the two ways of caluclating the discontinuity are consistent.

Finally it should be mentioned that both, the dispersion of the lowest peak in the spectral function for the annihilation of an electron and the $\mathbf{k}$ dependence of its residuum, can also be seen in exact diagonalization studies[17] where $|\Psi_0\rangle$ in (19) is replaced by the ground state of an 18-site cluster with two holes (this corresponds to a hole concentration of 11%). This may be viewed as an indication that even at such high doping the "string" picture still has a certain relevance.

IV. CONCLUSION

The momentum distribution function and the pole strength of the dominant pole in the one-hole spectral function for the t-J model have been evaluated. It was found that both quantities are not consistent with what one would obtain by simply filling the band obtained from the one-particle dispersion relation with holes. Rather both quantities show some features which are reminiscent of a Fermi liquid of weakly interacting quasiparticles whose one-particle energies are given by the tight-binding band calculated from the hopping term alone. A possible interpretation of this behavior is as follows: when a single hole is moving through an antiferromagnetically ordered spin background its motion can be described by a coherent superposition of localized states $|\Phi_j\rangle$, where the hole is bound to one particular site j by an effective potential due to strings. When the momentum distribution function for such a wave function is calculated one obtains two contributions: one of them is due to the motion of the "center" of the localized state, j, and this part depends on the total momentum of the "quasiparticle." In the framework of the rigid-band approximation this part will give the hole pockets which would be expected from the one-particle dispersion relation. The other contribution however is due to the motion if the hole "inside" the localized states $|\Phi_j\rangle$. This contribution might be viewed as some kind of "form factor." It turns out that it is precisely the contribution from this "form factor" which results in the similarity to free particles. One can understand this if one considers the limiting case of an extremely weak string potential. Then the wave function of the hole moving under the influence of the string potential will be rather similar to that of a free hole which does not feel any kind of sublattice structure. Therefore contributions which are due to the "internal structure" of the localized states may be expected to be qualitatively similar to that of free particles.

It should be noted that despite the fact that the ansatz wave function (4) has long-range Néel order this feature does not really enter the calculation. In fact the only conditions required in the above calculations are short-range Néel order (to produce the string potential) and translational invariance [to justify an ansatz like (4)]. A change of the dispersion relation due to deviations from the Néel order would change predominantly the position of the hole pockets but not so much the contributions due to the "form factor." Thus one might expect that for a translationally invariant "spin background" with sufficiently strong short-range antiferromagnetic spin correlations ("spin liquid") the above calculations still have some relevance. Thereby prefactors like $\alpha_1\alpha_2$ in (17) will certainly change due to the deviations from the Néel order. On the other hand the $\mathbf{k}$ dependence, for example, of the contribution (17) is determined by geometry, so it should remain the same.

Admittedly the similarity between the caluclated quantities and their behavior for free particles is at most qualitative. Especially within the framework of the present formalism one has nothing to say about the origin and the location of the "true" Fermi liquid discontinuity in the momentum distribution function which should appear at very high hole doping. One should always bear in mind however, that the momentum distribution function is particularly difficult to calculate from a "projected" Hamiltonian like the t-J model. Also it is very difficult to reproduce the Fermi surface singularity for free particles within the framework of a local representation like the one used above. Indeed even if one would evaluate the momentum distribution function for free electrons it would be impossible to reproduce the discontinuity at the Fermi surface by just taking into account a finite number of difference vectors l in the representation (11). Thus one might speculate that the "string picture" and the "Fermi liquid picture" for a small concentration of holes are just two different ways of looking at the same thing and thus the range of doping where the high-T_c materials are superconducting might be accessible both from the weak and the strong correlation limits.

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