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Dynamics of one hole in the t-J model

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We calculated the spectral function of a hole in the t-J model using a numerical method on a 4×4 lattice. A sharp quasiparticle peak is observed with an energy that is well approximated by $\Delta E=-3.17+2.83J^a$ (for $0.1\leq J\leq 1.0$, $t=1$) with $a=0.73\pm0.02$. This result suggests that the picture of a hole attached to the origin by a string may be valid in the Heisenberg model. The rest of the spectrum is not completely incoherent but it has a nontrivial structure, stemming from the excited states of the string. The bandwidth of the quasiparticle is discussed. Results for the Ising model are also presented.

The discovery of the new high-T_c superconductors[1] have renewed the interest in the study of two-dimensional (2D) Hubbard-like models. Recently, it has been found that the undoped materials can be understood very well using the 2D spin-$\frac{1}{2}$ Heisenberg model.[2] However, not much is known about these models when holes are introduced in the system. As a first step it is important to understand the behavior of one hole in an antiferromagnet using the t-J model.[3] Some of its properties are already known: For example, static quantities such as ground-state energies and dispersion relations have been evaluated using variational spin-wave approximations[4] and numerical techniques.[5,6]

What do we know about the dynamical properties of one hole in a Mott insulator? Previous studies are based on self-consistent diagrammatic approaches or moment expansion methods. Brinkman and Rice[7] showed that at $U=\infty$ in the Hubbard model the spectral function of a hole is incoherent. For finite U this situation may change as indeed happens in one dimension.[8] In 2D much progress has been made recently[9] in the context of the t-J model, where it was shown that a quasiparticle peak exists in the spectral function of a hole for finite J. Beyond that peak the rest of the spectrum is conjectured to be incoherent.[9]

Although these calculations are appealing, it is important to check their main predictions against numerical results. In principle there is no obvious small parameter controlling the convergence of the self-consistent method used in Ref. 9. However, a numerical calculation of spectral functions is very difficult. To measure properties of a system in real time using Monte Carlo methods, high accuracy in imaginary time observables is needed. A better way to proceed is by using Lanczos methods. In this case complex numbers can be easily handled and a calculation in real time is possible. Even more, spectral functions can be obtained[10–13] as mean values of appropriately chosen operators in the ground state of the system. Then there is no need to calculate the complete spectrum of the Hamiltonian.

In this Rapid Communication we present the first numerical study of the spectral function of one hole in the t-J model in 2D. This model is defined by the Hamiltonian

$$H=J\sum_{\mathbf{i},\hat{\epsilon}}\mathbf{S}_\mathbf{i}\cdot\mathbf{S}_{\mathbf{i}+\hat{\epsilon}}-t\sum_{\mathbf{i},\hat{\epsilon},\sigma}(\bar{c}^\dagger_{\mathbf{i},\sigma}\bar{c}_{\mathbf{i}+\hat{\epsilon},\sigma}+\text{H.c.})\,, \tag{1}$$

where the first term corresponds to a Heisenberg interaction among the spins while the second is an electron-hopping term acting with the constraint of no double occupancy (hole hopping). The notation is standard. We work on a two-dimensional square lattice with periodic boundary conditions. The operators $\bar{c}_{i,\sigma}$ correspond to hole operators. We consider $t=1$ in the rest of the paper.

To obtain information about the dynamics of this problem we introduce the spectral function of one hole with energy ω and momentum $\mathbf{k}$, defined as[12]

$$S(\mathbf{k},\omega)=-(1/\pi)\text{Im}[G(\mathbf{k},\omega+E_0+i\epsilon)]\,, \tag{2}$$

where

$$G(\mathbf{k},x)=\langle\psi_0|\bar{c}_\mathbf{k}(x-H)^{-1}\bar{c}^\dagger_\mathbf{k}|\psi_0\rangle$$

and

$$\bar{c}^\dagger_\mathbf{k}=\sum_\mathbf{i}\exp(i\mathbf{k}\cdot\mathbf{i})\bar{c}^\dagger_\mathbf{i}\,.$$

We consider hole operators with spin up (the spin index is dropped from now on). The state $|\psi_0\rangle$ is the ground state of the Heisenberg model in the absence of holes (with energy E_0) that we obtained using a modified Lanczos method.[14] ϵ is a small parameter that gives a finite width to the δ functions appearing at each pole of G. All possible states of the one-hole subspace having a nonzero projection over the state $|1\rangle=\bar{c}^\dagger_\mathbf{k}|\psi_0\rangle$ will contribute to the spectral function. G admits a continued fraction expansion since it has poles only on the real axis. The coefficients a_m,b_m of this expansion can be obtained from powers of H in the state of one hole $|1\rangle$ which are evaluated numerically for increasing m until convergence is observed.[13] As a check of our program we reproduced the ground-state hole energies previously obtained by Lanczos methods[5] and we also satisfied the standard sum rule coming from the integration over ω of the spectral function.

Our main results are the following: In Fig. 1 we show the spectral function of one hole at different values of J and for $\mathbf{k}=(\pi/2,\pi/2)$.[15] At $J=0$ there are no clear dominant peaks, although there is some structure superimposed on the incoherent background predicted in Ref. 7. Note the strong depletion near $\omega=0$ where there are states present but with very small spectral weight (pseudogap). Its existence produces two well-defined bands in the problem. In fact, the spectral function at $J=0$ and $\mathbf{k}=(\pi/2,\pi/2)$ is symmetric under $\omega \to -\omega$. This symmetry comes from a change in the sign of t when a (-1) is absorbed in the fermionic operators at even sites. The first pole at $J=0$ [Fig. 1(a)] is located at $\simeq -3.40$ which is close to the result -3.34 given by Joynt[16] and also to the result of Brinkman and Rice[7] $-2\sqrt{3}\simeq -3.46$. It is important to note that the state $|1\rangle$ has total spin $\frac{1}{2}$ so states with higher spin will not appear in our spectral function[17] (the "band tails" of Ref. 7).

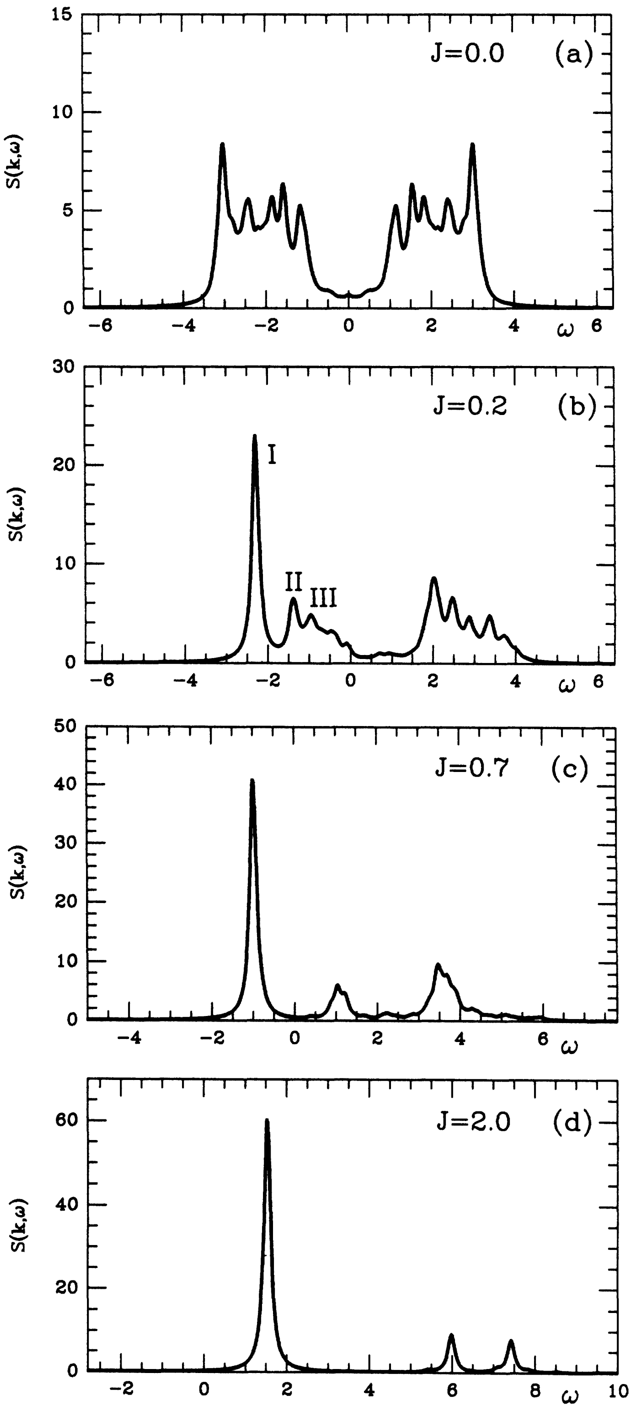

FIG. 1. Spectral function of one hole for different values of J on a 4×4 lattice [$t=1$, $\epsilon=0.1$, and $\mathbf{k}=(\pi/2,\pi/2)$].

At $J=0.2$ [Fig. 1(b)] the results have already changed drastically. Now a clear peak is present at the bottom of the spectrum corresponding to a quasiparticle. This peak is separated by a small gap from a band which shows some modulation. A pseudogap still separates this structure from a second band also presenting peaks on top of an incoherent spectrum. This additional band comes from the $\omega>0$ sector of the spectrum at $J=0$ and is a direct consequence of the pseudogap near $\omega=0$ that exists in that limit. Increasing J, three well-defined structures survive. For example, at $J=0.7$ [Fig. 1(c)] the two broad bands (found after the quasiparticle peak at small J), have appreciably reduced their width. At $J=2.0$ [Fig. 1(d)] only two small peaks can be observed besides the quasiparticle. However, note that although the total width of the spectrum seems to be $\approx 8t$, in fact there are many more poles at high energies (with very small spectral weight) than those that can be observed in Fig. 1.[18]

To understand our results we studied the energy of the quasiparticle versus J. This energy ΔE can be fitted with high accuracy by a power law as $\Delta E=-3.17+2.83J^{\alpha}$, where $\alpha=0.73\pm0.02$ for intermediate values of $J (0.1 \leq J \leq 1.0)$ (for very large J all the levels scales as J as expected). In addition, we also found (in the same interval of J) that the energy of the second peak [denoted by II in Fig. 1(b)] is also well approximated by $\Delta E=-3.13+5.36J^{\alpha}$ where $\alpha=0.70\pm0.04$.[19]

These results can be understood as follows, by analogy to the Ising case.[20] A local wave function for the hole, analogous to a Wannier function in a single-particle tight-binding model, can be constructed by allowing the hole to move on its string away from a central site. We find a linear potential equal to $2(-d_1+d_2)Jl \approx 1.1Jl$ where d_1 and d_2 are the first- and second-neighbor spin-correlation functions of $|\psi_0\rangle$, and l is the length of the string. The theoretical prediction for the energy of the lowest-hole state is $\Delta E=-3.34+2.93J^{2/3}$, in good agreement with our numerical results and also with the results in the Ising limit[20] $\Delta E=-3.46+2.74J^{2/3}$. The subsidiary peaks can be identified as excited states of the hole on the string by the J dependence of their energies. The spin fluctuations are not fast enough to destroy the string which lasts for a time $\sim 1/J$. By comparing this time to the time needed for a hole to reach its classical turning point in the linear potential, one finds two bound states of the string for $J=0.2$. This qualitative argument tells us to expect some additional structure in the low-energy spectrum, as observed. The number of bound states predicted by this argument is $\sim 1/J$ as $J \to 0$.

As a further test of these ideas, note that for very small J all the levels of the string should converge to the same value. This is in excellent agreement with the behavior of the first and second peaks extrapolated to $J=0$ $(-3.17$

and -3.13, respectively) (see Fig. 2). The intensity of the other peaks quickly diminishes with J. The fact that numerically at $J=0$ there still exist peaks in our results can be attributed to the finite size of the lattice. In fact, this effect can also be understood from the string picture where we find that the average length of the string behaves as $1.43/J^{1/3}$, which is equal to 4 (the size of our lattice) for $J\approx 0.05$. So although in principle our calculations on a 4×4 lattice may be affected by finite-size effects, the analysis of the size of the ground state and its energy show that they are not very important.

In addition to the main peaks there are many other peaks of lower intensity. Those are probably due to spin-wave excitations. For the Heisenberg model without holes we found (for a 4×4 lattice) that the spin-wave energy (with respect to the ground state) ranges from $0.58J$ at $\mathbf{k}=(\pi,\pi)$ to $2.71J$ at $\mathbf{k}=(\pi/2,\pi/2)$. These energies are of the correct order of magnitude to explain part of the spectrum shown in Fig. 1. Note also that the second broad band observed in Fig. 1(b) cannot be accommodated in the string picture (only the first few levels admit such an interpretation because the rest are unstable as was shown above). It would be very interesting to understand analytically the origin of this new band.

What is the dispersion relation of the quasiparticle? We evaluate it by calculating the position of the dominant peak for different values of $\mathbf{k}$. The bandwidth is defined as the difference in energy between the quasiparticle states with maximum and minimum energy.[21] We found that the state with highest energy corresponds to $\mathbf{k}=(0,0)$ while the minimum is at $\mathbf{k}=(\pi/2,\pi/2)$ as expected.[22] For $0.2\le J\le 0.6$ we can fit the state of minimum energy in the sector of $\mathbf{k}=(0,0)$ as $\Delta E\approx -3.5+4.7J^{0.7}$ (similar results were found for all the possible values of $\mathbf{k}$). Combining the results for $\mathbf{k}=(0,0)$ and $\mathbf{k}=(\pi/2,\pi/2)$ we conclude that the bandwidth in this region behaves approximately as $J^{0.7}$. (A calculation is in progress to check if this result is also in agreement with the string picture or not.) Then, although we fully agree with Ref. 9 that there is a drastic reduction in the bandwidth from t to J^{α}, we do not agree in the exponent, at least for $0.2<J<0.6$. They obtained $\alpha=1$ in the dominant pole approximation while our numerical results suggest $\alpha\approx 0.7$. (Recently a strong nonlinearity in a new Green's-function approach was found[23] suggesting that spectral weights do not scale as J for $J>0.01$.) We also found analytically and numerically that for $J\gg t$, the bandwidth is proportional to t rather than t^2/J as in the Ising model.[24]

In Fig. 3 we show results for the t-J_z model (Ising limit) at two values of J and $\mathbf{k}=(\pi/2,\pi/2)$. In this case the ground state for zero holes is the Néel state. The result for $J=0$ [Fig. 3(a)] does not have the depletion at $\omega=0$ observed in Fig. 1(a). The reason is that in the Ising limit the total spin is no longer a good quantum number (only S_z is conserved). So the spectral function will contain more peaks than in the Heisenberg limit (where we studied only the $S=\frac{1}{2}$ sector). In particular there will be states that correspond to the $S_z=\frac{1}{2}$ component of states of high spin in the Heisenberg model (this idea has been verified on a 2×2 lattice). Thus we conjecture that the peak at $\omega=0$ in Fig. 3(a) is due to ferromagnetic states, since this is where the free-particle pole would lie.

At $J_z=0.4$ [Fig. 3(b)] there is already a clear quasiparticle peak in the spectrum of the Ising model. Recently, using lattices of up to 8×8 sites, it has been found[25] that its energy scales like $-3.66+2.96J_z^{\alpha}$ with $\alpha=0.66\pm 0.02$ for $0.2\le J_z\le 1.0$ in excellent agreement with the string picture. (It is also remarkable that the results for the 4×4 lattice were already in close agreement with the final results of the 8×8 lattice showing that indeed the finite-size effects of our calculation are small). At $J_z\ge 2.0$ we found a result similar to that of Fig. 1(d) for the Heisenberg model. For the Ising limit we can do a good quanti-

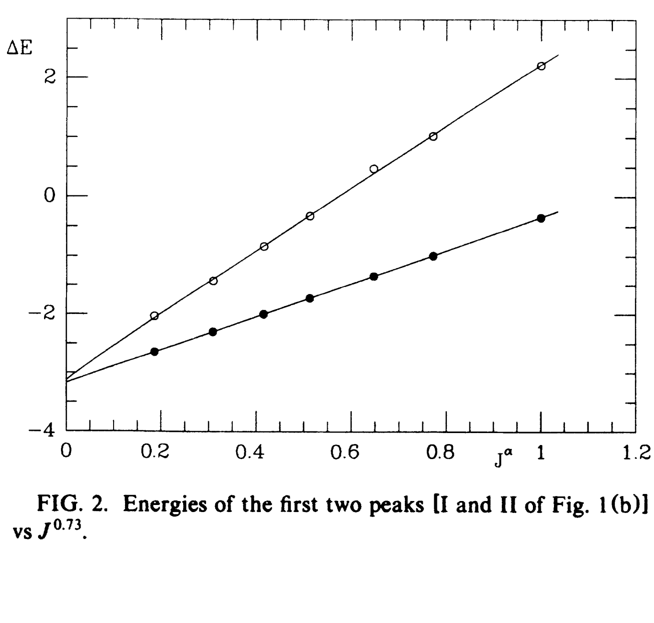

FIG. 2. Energies of the first two peaks [I and II of Fig. 1(b)] vs $J^{0.73}$.

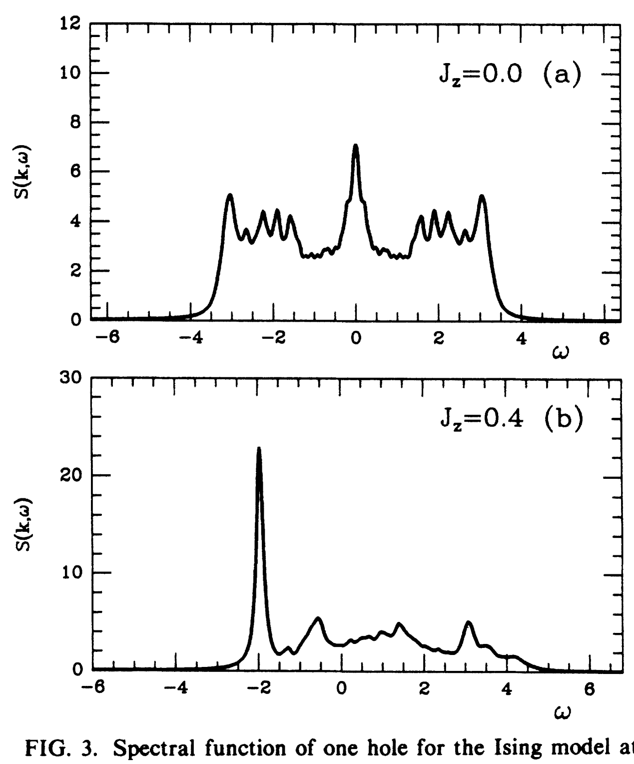

FIG. 3. Spectral function of one hole for the Ising model at $J=0.0$ and 0.4 on a 4×4 lattice [$t=1$, $\epsilon=0.1$, and $\mathbf{k}=(\pi/2,\pi/2)$].

tative analysis and we found that the quasiparticle peak corresponds to the hole (static) at a given site while the first peak is the hole moving one lattice spacing in any direction (in fact, many other low intensity peaks were identified in the Ising limit). We believe that a similar situation occurs for the Heisenberg model and that the first two levels found in Fig. 1(d) (presumably with a string of length 0 and 1, respectively) are smoothly connected to the first two levels of the 1D confining problem described above for small J. We also remark that the position of the quasiparticle peak in the Ising limit is not $\mathbf{k}$ independent, perhaps due to the high-order processes mentioned by Trugman.[4] However, the bandwidth is very small showing that the influence of these processes can be safely neglected.

Additional details will be presented elsewhere. A study of larger lattices is in preparation (preliminary results for an 18 site lattice do not show drastic changes in our results). Upon completion of this work we learned that Trugman[26] is also calculating $S(\mathbf{k},\omega)$ using a different technique. We also know that other groups[27,28] are working along similar lines.

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[15] $\mathbf{k}=(\pi/2,\pi/2)$ is the momentum of the hole that minimizes the energy in the antiferromagnetic region (Refs. 4–6). For very small J the ground state is actually ferromagnetic (Nagaoka theorem). However, our results always correspond to the subspace of spin $\frac{1}{2}$.

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[17] For example, the saturated ferromagnetic state with energy $-4t$ which is the real ground state at $J=0$ is not present here since it is orthogonal to $|1\rangle$. Only states with a nonzero overlap with $|1\rangle$ contribute to the spectral function.

[18] The results of Fig. 1 have been obtained with many iterations of the continued fraction expansion (typically between 100 and 300 until convergence was observed) so in principle many poles can be generated. In fact, repeating the calculation of Fig. 1 with $\epsilon=0.01$ instead of $\epsilon=0.1$, the individual peaks can be seen clearly. In addition to the dominant peaks there are many others (hundreds) of lower intensity.

[19] A third peak [III in Fig. 1(b)] can be distinguished from the background in a narrow interval of $J(0.2\leq J\leq 0.4)$ and its energy behaves as $\Delta E=-3.23+6.26J^{0.63}$. Note that the slopes we found in the fit ΔE vs J^{α} (i.e., 2.83, 5.36, and 6.26) are in good correspondence with the first eigenvalues of the Airy equation (i.e., 2.33, 4.08, and 5.52), especially taking ratios. In fact even the first peak located after the broad pseudogap also seems to follow a power-law behavior with α close to 0.7 (although with bigger error bars). This peak is particularly interesting since its intensity is high compared to the rest and it behaves like a quasiparticle itself for small J (although with a finite lifetime).

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[21] Special care must be taken for $\mathbf{k}=(0,0)$ because we found that the ground state in this sector is orthogonal to the state $|1\rangle$. Such a problem can be clearly seen on a 2×2 lattice where exact solutions are obtained analytically. In that case the ground state at $\mathbf{k}=(0,0)$ is odd under a rotation in $\pi/2$ while $|1\rangle$ is even. Nevertheless the energy for $\mathbf{k}=(0,0)$ can be evaluated using some other method like the Lanczos technique.

[22] This occurs for intermediate values of J. In addition to the crossing of levels at very small J due to the Nagaoka theorem the t-J model presents additional crossings at large J. For example, at $J>2$ the energy is minimized by $\mathbf{k}=(\pi/2,\pi)$ and for even larger values of J there is an additional crossing of levels with the minimum now at $\mathbf{k}=(\pi,\pi)$.

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