

ONE HOLE SPECTRAL DENSITIES IN THE POLARIZED t - J MODEL

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Abstract

We study the dynamics of one hole in the polarized t - J model. The model describes the physics of holes in polarized antiferromagnetic systems and the one particle excitations in strong coupling superconductors as well. The spectral densities of a single hole are calculated numerically using exact diagonalization of small clusters with toroidal boundary conditions. The quasiparticle spectrum is analyzed in detail. We show that a coherent quasiparticle peak is well defined for $J/t > 0.2$. The dispersion relation of the quasiparticle is obtained for different magnetizations. The results are used to discuss the characteristics of one particle excitations in small coherence-length superconductors.

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I. Introduction

Since the discovery of high T_c superconductors, much effort has been devoted to the study of low-dimensional electronic systems, in particular, the one band and two band Hubbard models. These models have been extensively studied in the strong coupling regime ($U \gg t$). In this limit, the one band Hubbard model can be mapped onto the so called t - J model.¹ This mapping is however approximate: second nearest neighbour hopping terms of the order t^2/U are neglected. The t - J Hamiltonian is believed to contain the relevant physics for high T_c superconductivity and has been widely used in this context²⁻⁴. Perhaps the main reason for the study of this model is its simplicity together with the fact that it contains what is considered the essential ingredients for the understanding of high T_c materials: charge and spin excitations in different energy scales. For one electron per site, the model reduces to the Heisenberg model where only spin excitations are possible. This case corresponds to the Mott insulating regime of the original Hubbard model. For less than one electron per site, charge excitations become important.

Resorting to different approximations a number of analytical approaches have been reported for the ground state properties of a single hole⁵⁻⁷. Shraiman and Siggia found, using a variational method and spin wave techniques, that the momentum of the hole is $k=(\pm\pi/2, \pm\pi/2)$ which lies on the Fermi surface of the non-interacting ($U=0$) system. Analogous results have been obtained

using variational and diagrammatic techniques and numerical exact diagonalization^{8,9} Also, dynamical properties have been reported using numerical techniques. These results show that for $J \approx t$ a well defined quasiparticle peak is identified, whereas for small enough J/t an incoherent spectrum carries most of the spectral weight. These studies are concerned with the movement of a hole in an antiferromagnetic background. On the other hand, some work has been done to obtain the spectral densities $\rho(k, \omega)$ in the phase with no antiferromagnetic long-range order, i.e. the spin liquid phase.¹¹ Unfortunately the numerical simulations in the spin liquid phase are difficult to handle, which does not allow to check the conjectures made.

Recently another realization of the t - J model has been devised in connection with one particle excitations of strong coupling superconductors with local attraction.¹² It is well known that the negative U Hubbard model with n particles is equivalent to the positive U case with one particle per site and a net magnetization per site given by $S_z = (1-n)/2$.¹³ The dynamics of a single unpaired particle moving in the background of strongly bounded paired particles is described by the polarized t - J model.

The main purpose of the present work is to describe the dynamics of holes in the polarized t - J model. We interpret our results either as corresponding to a conventional t - J model with an additional parameter (an external magnetic field) or to the case of a single one particle excitation in the strong coupling

superconductor mentioned above. The results presented below are obtained by exact diagonalization of finite clusters.

The rest of the paper is organized as follows. In section II we present the model. In section III we present the obtained results, and section IV includes a summary and discussions.

II. The model

The starting point is a Hubbard model with on-site interactions only and a nearest neighbor hopping matrix element. We consider a square lattice in 2D. The Hamiltonian in the usual notation reads

$$H = -t \sum_{\langle i,j \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (1)$$

where $c_{i\sigma}^\dagger$ creates an electron with spin σ at site i and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. The parameters t and U are respectively the hopping matrix element and the in-site interaction. We consider the case $|U| \gg t$ and site occupation $n \leq 1$. For positive U (repulsive case) a canonical transformation which projects out the doubly occupied sites can be performed to obtain the t - J model, which is given by

$$H = -t \sum_{\langle i,j \rangle \sigma} (1-n_{i-\sigma}) c_{i\sigma}^\dagger c_{j\sigma} (1-n_{j-\sigma}) + J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + \frac{1}{4} \sum_i n_i n_i + H' \quad (2)$$

Here the hopping term describes the jump of an electron in the projected Hilbert space which excludes doubly occupied sites. The second term describes the antiferromagnetic coupling between the spins of electrons in singly occupied nearest-neighbor sites.

The coupling constant J is given by $J=4t^2/U$. Finally, the last term H' , which is usually neglected describes second nearest neighbor hopping of the order t^2/U with and without a spin flip process. In what follows, we also neglect this term. We add to the t - J model an external magnetic field h which polarizes the spins.

On the other hand, for large negative U , an analog procedure can be carried out. In fact, the negative U Hubbard model can be mapped onto the positive U Hubbard model with an external magnetic field. Instead of making use of this transformation, which is valid for arbitrary U , we consider the large $|U|$ limit and project out the singly occupied states. This leads to the following Hamiltonian¹⁴

$$H = J \sum_{\langle i,j \rangle} S_i^z S_j^z - \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+) - h \sum_i S_i^z \quad (3)$$

Now, the spin variables up and down correspond to an empty and a doubly occupied site respectively. The longitudinal antiferromagnetic term describes a repulsion between nearest neighbor pairs while the ferromagnetic transverse term describes a hopping of a pair through virtual pair breaking processes. The external magnetic field h plays the role of a chemical potential since the total magnetization is given by the total number of particles, $S^z = \frac{1}{2}(1-n)$. The strength of the coupling is again $J=4t^2/|U|$. This spin Hamiltonian is equivalent to a purely antiferromagnetic Heisenberg model. This can be seen by performing a rotation in π around the z axis for a given sublattice. This

changes, in one sublattice, S^x and S^y by $-S^x$ and $-S^y$, and consequently the sign of the transverse term. In this spin language, states with long range magnetic order can be identified with a superfluid phase of the original electron system, the superfluid order parameter being the magnetization in the x-y plane. The orientation of $\langle S^+ \rangle$ is the phase of the superfluid order parameter. On the other hand, the paramagnetic spin state corresponds to the normal state of the bound electrons system with no phase coherence between the pairs (or spins, depending on the language used).

Some insight on the background distortion caused by the motion of a single unpaired particle can be gained if one analyzes the classical limit in which the spin fluctuations are suppressed. In this limit, the ground state of the spin system alone corresponds to spins tilted with respect to the z axis in such a way to satisfy the constraint of fixed magnetization. The order of the projected components in the x-y plane depends on whether one uses the ferromagnetic or the antiferromagnetic description. If the ferromagnetic description of Hamiltonian (3) is used, the ground state in the classical limit, and in the electron description is given by¹²

$$|\phi_0\rangle = \prod_l (u + v c_{l\uparrow}^\dagger c_{l\downarrow}^\dagger) |0\rangle \quad (4)$$

The system described above with a single unpaired electron can be mapped as follows onto the ordinary t-J model. It is

convenient to divide the Hamiltonian into two terms, H_j and H_t . The first term is $H_j = \sum_i H_j(i)$, where $H_j(i)$ describes the spin dynamics with the unpaired particle located at site i . The zero point fluctuations will distort the superfluid order parameter in the neighborhood of the unpaired electron, in analogy with a fixed hole in the Heisenberg model. The second term H_t describes the hopping of the unpaired electron. When the electron jumps from site i to site j , a tilted spin, which corresponds (in the electron language) to a linear combination of empty and double occupation jumps backwards from site j to site i . In this process the z component of the spin is conserved. The phase in the x - y plane changes. This is clearly seen in the classical limit, where the initial and final states ($|\psi_i\rangle$ and $|\psi_j\rangle$ respectively) are given by

$$|\psi_i\rangle = c_{i\sigma}^\dagger \prod_\ell (u + v c_{\ell\uparrow}^\dagger c_{\ell\downarrow}^\dagger) |0\rangle \quad (5)$$

and

$$|\psi_j\rangle = c_{j\sigma}^\dagger (u - v c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger) \prod_{\ell \neq i} (u + v c_{\ell\uparrow}^\dagger c_{\ell\downarrow}^\dagger) |0\rangle \quad (6)$$

the change in sign in the coherent factor of site i , corresponds in the spin language to a change in the x - y component of the spin. If the antiferromagnetic picture is used, both the z -component and the phase in the x - y plane are conserved.

To summarize the discussion made above, we consider the

polarized t-J model which can be used to study the motion of a hole in a polarized antiferromagnetic background or the single particle dynamics in a superconductor with strong on-site attraction.

In the next section we present results for the frequency dependent correlation function $\rho(k, \omega) = \langle \psi_0 | \tilde{c}_{k\sigma}(t) \tilde{c}_{k\sigma}^+ | \psi_0 \rangle$, where $|\psi_0\rangle$ is the ground state wave function of the polarized Heisenberg Hamiltonian, $\tilde{c}_{k\sigma}^+$ creates a particle and the subindex ω indicates a Fourier transformation. In the case of the positive U Hubbard model $\tilde{c}_{k\sigma}^+$ creates a hole of spin σ i.e. destroys one of the spins of the lattice with $S_z = \sigma$. In the presence of an external magnetic field which polarizes the system the correlation function $\rho(k, \omega)$ depends on the spin σ . If we use the model to describe single particle excitations in a strong coupling superconductor, $\tilde{c}_{k\sigma}^+$ creates an electron which will move in the presence of the strongly bound pairs. In this case spin up and spin down electrons will behave in the same way. The extra particle can be created only in the empty sites or, in the spin language, in sites occupied by a spin up. If we calculate $\rho(k, \omega)$ corresponding to a hole in the Heisenberg model, to obtain the spectral density of an electron in the superconducting background we have to take $\sigma = \uparrow$ and change k by $\pi - k$. The change in the vector wave number k is due to the fact that in one picture $\tilde{c}_{k\sigma}^+$ creates a hole while in the other it creates an electron. If we consider the fully polarized state with $M=1/2$ all many body effects disappear and the minimum energy

for a hole corresponds to $k=(\pi,\pi)$. In the negative U case, this state represents the vacuum and the minimum energy for an electron added to the vacuum corresponds to $k=(0,0)$.

III. Numerical results

The starting point of the calculation is to obtain the ground state wave function $|\psi_0\rangle$ of the Heisenberg Hamiltonian for different magnetizations M . The effect of the external magnetic field h is just a shift of the energy given by $-hM$. In Fig. 1 we show the energy spectrum of the Heisenberg model as a function of the magnetic field h for a small (4x4) cluster. As can be seen in the figure there is always a range of magnetic field which stabilizes a given magnetization. In what follows instead of working with a magnetic field h we fix a magnetization and neglect the magnetic shift $-hM$.

We study the one hole spectral function for all possible values of k consistent with our cluster with periodic boundary conditions, for $0 \leq J/t \leq 1.5$ and all magnetizations. The numerical results are obtained for a small cluster of 4x4 sites using the methods described in Ref.15. Most of the results presented in this section correspond to a spin up hole. The case of a spin down hole can be obtained from the previous one by reversing the magnetization. In the next section we reinterpret these results in terms of a single particle excitation in the negative U Hubbard model.

The numerical results show that, in all cases, for $J/t > 0.2$, a quasiparticle peak can be identified as the lower energy peak in the spectral function which can be distinguished from the incoherent part. For a finite system the incoherent part is not a continuum of states but it consists of a set of delta functions more or less close to each other. The finiteness of the system therefore makes the definition of quasiparticle a meaningless concept for intermediate situations where a peak cannot be clearly distinguished from the rest of the spectrum.

In Fig. 2 we present results for the spectral functions $\rho(k, \omega)$ corresponding to $k=(\pi/2, \pi/2)$, for $J=0$ and different magnetizations $M=(N_{\uparrow}-N_{\downarrow})/2N$; N_{σ} and N are the number of spins with z component equal to σ and the total number of sites respectively. For the unpolarized situation, the results agree with those presented in Ref.8. In this case, the spectral density presents two bands separated by a pseudogap at $\omega \approx 0$. As the magnetization increases some peaks appear in the pseudogap region. In particular for the fully polarized state the spectral density presents a single line centered at $\omega = 0$. These results confirm the conjecture made in Ref.8 where the peaks obtained for $\omega \approx 0$ in the Ising limit were associated to high spin components of the wave function. For $J = 0$ no quasiparticle line (except in the fully polarized case) can be clearly distinguished and the spectrum is probably completely incoherent for all magnetizations ($|M| < 1/2$). This is in agreement with the analytical results obtained in

Ref.12. If the spectrum is completely incoherent the total width of the spectral density $\rho(k,\omega)$ for any value of k coincides with the total bandwidth of the hole. For the unpolarized system and $k=(\pi/2,\pi/2)$, $\rho(k,\omega)$ extends from $\omega \approx -3.4t$ to $\omega \approx 3.4t$. As the magnetization increases, the support of $\rho(k,\omega)$ increases and for large magnetizations it goes from $\omega \approx -4t$ to $\omega \approx 4t$. This result agrees with the Brinkman and Rice analysis.⁵ They showed using the self retracing path approximation that the bottom of the incoherent band is at $\omega = -2\sqrt{3} t$. This is in agreement with the results obtained for $M=0$ where the total spin of the system with the hole is $S=1/2$. By increasing the magnetization, the total spin increases and the bottom of the incoherent band shifts towards lower values reaching $-4t$ for the completely polarized system.

As J increases the spectral density changes and gives rise to a well defined quasiparticle peak. This is clearly shown in Figs. 3, 4, and 5 where we present the results for $k=(\pi/2,\pi/2)$, and different values of J and magnetization. As can be seen in the figures, for all magnetizations, by increasing J the quasiparticle peak increases in intensity and separates from the incoherent spectrum. For the unpolarized system the dispersion relation of the quasiparticle peak has a minimum for $k=(\pi/2,\pi/2)$. The energy of this peak as a function of J goes as J^α with $\alpha \approx 0.73$ ¹⁰. This result can be interpreted in terms of strings created by the hole as proposed in Ref.5 and discussed in some detail in Ref.10.

For the polarized system, as we show bellow, the minimum

energy of the quasiparticle is no longer at $k=(\pi/2, \pi/2)$. For all k 's the behaviour of the spectral function is qualitatively the same. For small J the quasiparticle line carries a small weight which increases as J increases. As an example, in Fig.6 we present results for $k=(0,0)$ and $M=-0.25$. Note that in this case the spectral density has less structure than for $k=(\pi/2, \pi/2)$.

The energy of the quasiparticle peak for different magnetizations as a function of k is shown in Fig.7. The energies of both spin up and spin down holes are shown. For $k \neq (0,0)$ the spin up hole, i.e. a hole in the majority spin subspace, has always smaller energy than the spin down hole. This can be interpreted as an indication that for $J/t=0.2$ the energy of the state with one hole is smaller if the total spin is smaller. It has been shown that the Nagaoka state, which corresponds to the stabilization of the ferromagnetic state by introducing a hole to the system, occurs in our small cluster only for $J/t < 0.075$. For $k=(0,0)$ we always find degeneracies between the energies of the quasiparticles with majority and minority spins. This is probably due to the fact that for this value of k the total spin of the system with one hole is not given by the minimum total spin compatible with S_z .

The results of Fig 7 can be summarized as follows: For the highly polarized system a hole with spin σ equal to the majority spin leads to a narrow quasiparticle band with the minimum at $k=(\pi, \pi)$. This band shape resembles the case of the fully polarized

situation although the band width is much smaller. As the magnetization decreases the bandwidth decreases and the minimum shifts towards $(\pi/2, \pi/2)$. For zero magnetization the minimum reaches $(\pi/2, \pi/2)$ and the dispersion relation is similar to that of a particle moving in a lattice which has doubled its periodicity. In the present calculation, however, the degeneracy between the points $k=(\pi/2, \pi/2)$ and $k=(\pi, 0)$ is due to a finite size effect as discussed in Ref. 10.

It is interesting to analyze the weight of the quasiparticle line. In all cases the quasiparticle peaks corresponding to k 's close to the bottom of the band have more weight than those corresponding to the top of the band. For the k 's at the top of the quasiparticle band the weight can be very small even for intermediate values of J/t . To illustrate this behaviour, we show in Fig. 8 the spectral densities $\rho(k, \omega)$ for different values of k . For these parameters, the quasiparticle peak corresponding to the k of the bottom of the quasiparticle band carries 0.22 of the total spectral weight. For the k at the top of the band the weight of the quasiparticle peak is 1.66×10^{-3} . In this last case the concept of quasiparticle becomes somewhat meaningless. In any case, at the bottom of the band the quasiparticle peak is well defined for intermediate or large values of J/t .

The value of k corresponding to the bottom of the band as a function of magnetization is shown in Fig. 9 for $J/t=0.2$ and 1. For $M=0$ we indicate the minimum at $k=(\pi/2, \pi/2)$ rather than $k=(0, \pi)$

since the energy of the former is probably the absolute minimum in the larger system. As the magnetization increases ($M>0$) the values of k shift towards (π, π) . This shift is more abrupt for large values of J . This part of the curve corresponds to destroying a majority spin and the results agree with the analytical results presented in Ref.12. For $M<0$ the values of k corresponding to the bottom of the band shift towards the center of the zone in a similar way.

The total bandwidth of the quasiparticle as a function of J and magnetization is shown in Fig.10. For high magnetizations the bandwidth grows linearly with J for the range of J/t studied ($0.2 < J/t < 1.5$). As the magnetization decreases the increase in the total bandwidth deviates from the linear behaviour and for $M=0$ the total bandwidth goes like J^α with $\alpha=0.7$. For a given value of J the total bandwidth of the quasiparticle, which is a measure of the inverse of its effective mass, increases as the magnetization increases. We may picture out the quasiparticle as the hole dressed by spin fluctuations; as the magnetization increases spin fluctuations are partially suppressed and we expect the effective mass of the quasiparticle to decrease as the numerical results indicate.

IV. Summary and Conclusions

We have studied the spectral function for one hole in the polarized t - J model. Most of the results presented in the previous

sections correspond to a spin up hole i.e. the spectral densities $\rho(k, \omega)$ describes the dynamics of a hole obtained by destroying a spin up electron from the spin wave function $|\psi_0\rangle$ of the Heisenberg Hamiltonian.

The results can be summarized as follows:

The spectral density $\rho(k, \omega)$ for $k=(\pi/2, \pi/2)$ and $J=0$ is completely incoherent for all magnetizations, except for the fully polarized system ($M=1/2$). For $M=0$ the spectral density presents two bands separated by a pseudogap at $\omega \approx 0$. The total bandwidth extends from $\omega \approx -3.4t$ to $3.4t$ in agreement with the self retracing path approximation of Brinkman and Rice.⁵ As the magnetization increases, some peaks appear in the pseudogap. This confirms the conjecture of Ref.8 where the peaks obtained at $\omega \approx 0$ in the Ising limit (the $t-J_z$ model), were attributed to high spin configurations. The total bandwidth of the spectral density increases with magnetization reaching $8t$ for $M=1/2$. In this limit ($J=0$) the qualitative behavior of $\rho(k, \omega)$ is similar for all values of k : the spectrum is completely incoherent and the bandwidth increases with M .

For J larger than $0.2t$ there is a well defined quasiparticle peak at least for those k 's close to the bottom of the quasiparticle band. In all cases, for all magnetizations and k 's, the amplitude of the quasiparticle peak increases as J increases and separates from the incoherent spectrum. The quasiparticle band is always narrow, except in the fully polarized case, and its

minimum shifts with the magnetization. For spin up holes the minimum shifts from $k=(\pi/2, \pi/2)$ to $k=(\pi, \pi)$ as the magnetization increases from $M=0$ to $M=1/2$. Conversely the bottom of the band for the minority spin hole shifts from $k=(\pi/2, \pi/2)$ to $k=(0, 0)$.

If these results are used to describe the dynamics of an electron in a strong coupling superconductor with local interactions, the magnetization plays the role of the superconducting electron density. For low or intermediate densities ($M < 1/2$) the quasiparticle peak corresponding to the dressed electron forms a narrow band with its minimum energy for a value of k near the center of the Brillouin zone. It reaches the point Γ only in the limit of zero density. For a half filled band the minimum is located at the point $\Sigma=(\pi/2, \pi/2)$. However, for this case the superconductivity competes with the charge density wave state, an effect that we have not considered.

A single electron moving in a strong coupling superconductor is dressed by the superconducting fluctuations giving rise to a heavy quasiparticle which is, essentially, a particle in a so called pairing bag^{16, 17}. The size of the bag is a function of the pair-pair coupling J . The size of the bag decreases as J increases. In the present case, where all the calculations were done in a finite cluster, we expect important finite size effects for very small values of J . We stress that although the superconducting order parameter is depressed in the neighbourhood of the particle, in analogy with the depletion of the magnetic order parameter for

the case of a hole in an antiferromagnet, the pairing is not weakened. In the present strong coupling case, the energy needed to break a pair is always U , only the phase of the order parameter is distorted in the surroundings of the unpaired electron. In this sense, the denomination *pairing bag* is not appropriate to describe this strong coupling limit.

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Figure captions

- 1) Energy of the Heisenberg model vs. external magnetic field for different magnetizations. The slope of the curves are proportional to the magnetization of the system.
- 2) Spectral functions for $J=0$, $k=(\pi/2,\pi/2)$ and different magnetizations: a) $M=0$; b) $M=-1/8$; c) $M=-1/4$ and d) $M=-3/8$.
- 3) Spectral functions for $M=0$, $k=(\pi/2,\pi/2)$ and different values of J : a) $J=0.4$; b) $J=0.7$ and c) $J=1$.
- 4) Same as Fig.3 but with $M=-1/8$.
- 5) Same as Fig.3 but with $M=-1/4$.
- 6) Spectral functions for $M=-1/4$ and $k=(0,0)$ for: a) $J=0$; b) $J=0.2$; c) $J=0.4$ and d) $J=0.7$.
- 7) Dispersion relations for different magnetizations. The full line corresponds to a hole with spin σ equal to the minority spin of the system and the broken line to a hole with the majority spin. a) $M=-3/8$; b) $M=-1/4$; c) $M=-1/8$ and d) $M=0$. The points on the x -axis correspond to $k=(0,0)$, $(\pi/2,0)$, $(\pi,0)$, $(\pi,\pi/2)$, (π,π) and $(\pi/2,\pi/2)$ respectively. The circled point in a) has zero weight in the spectral density and was obtained by exact diagonalization.
- 8) Spectral functions for $M=-1/8$ and $J=0.7$: a) $k=(\pi/2,0)$; b) $k=(\pi,\pi)$.
- 9) The value of k corresponding to the bottom of the band as a function of magnetization for different values of J . Crosses: $J=0.2$; squares: $J=1$. The values of k are described in

Fig.7 .

- 10) Width of the quasiparticle band vs. J for different magnetizations: a) $M=0$; b) $M=1/8$; c) $M=1/4$; d) $M=3/8$.

















