Possible observation of “string excitations” of a hole in a quantum antiferromagnet

Efstratios Manousakis
Department of Physics, Florida State University, Tallahassee, FL 32306-4350
and Department of Physics, University of Athens, Greece.
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We argue that recently reported high resolution angle-resolved photoelectron spectra from cuprates, where an anomalous high-energy dispersion was identified, reveal the internal structure of the hole quasiparticle in quantum antiferromagnets and more importantly it is evidence for the existence of “string-excitations” which validate early predictions based on the $t-J$ model. Their energy-momentum dispersion as well as the in which the spectral weight is transferred to higher energy string excitations as well as the vanishing of the quasiparticle spectral weight near the $\Gamma$ point, are all in agreement with predictions without adjusting any parameters.

The study of the motion of a single hole in a quantum antiferromagnet is of general theoretical and experimental importance not only because it might be pertinent to the mechanism of superconductivity in the cuprates, but also because it is relevant to the field of quantum magnetism and strongly correlated systems, and has connections and analogies with the problem of impurity motion in antiferromagnets and in quantum solids and quantum liquids.

There is a solid body of angle-resolved photoelectron spectroscopy (ARPES) studies which reveal important features of the insulating, lightly doped, and overdoped cuprates. Here, we focus first on ARPES studies of the single hole dispersion in an undoped insulating antiferromagnetic parent compound. Early such studies demonstrated that there is a sharp well-defined quasiparticle-like peak in the spectral function which as function of momentum defines a band with a minimum near $(\pi/2, \pi/2)$ and a characteristic bandwidth approximately $2.2J$, where $J$ is the antiferromagnetic coupling. These features had been predicted by a number of studies of the hole motion in a quantum antiferromagnet in its simplest conception where a hole hopping term is added to the Heisenberg antiferromagnetic Hamiltonian, the so-called $t-J$ model. A deficiency of the simple $t-J$ model is that for momentum near $(\pi, 0)$ it gives a spectral function similar in shape and energy to that at $(\pi/2, \pi/2)$, while the ARPES measurements revealed that the quasiparticle peak is broader near $(\pi, 0)$ and the corresponding energy is higher than that at $(\pi/2, \pi/2)$. This discrepancy can be removed by adding relatively small direct next-nearest-neighbor hopping terms ($t'$ and $t''$) in the $t-J$ model.

However, in recent ARPES studies, high resolution data, taken along the $(0, 0)$ to $(\pi, \pi)$ cut, show an additional dispersive feature at higher energies that merges with the above mentioned band at lower energies. The main point of the present paper is to argue that these high resolution ARPES studies have revealed the internal structure of the single-hole quasiparticle as well as the existence and the energy-momentum dispersion of “string excitations”.

When a quantum hole is created in a classical antiferromagnet (such as, the $t-J$ model), the hole stays bound to its “birth-site” due to a “string” of overturned spins produced by the hole motion in its attempt to compromise its uncertainty in momentum by allowing for some position uncertainty. In a quasi-continuum picture, the hole is trapped by a linearly rising potential characterized by energy eigenstates, the so-called Airy functions, with energies $E_n/t = \epsilon_n + a_n(J_z/t)^{2/3}$, and the average length of the string scales as $(t/J_z)^{1/3}$ (here $t$ is the hole-hopping matrix element and $J_z$ is the coupling along the $z$ direction in spin-space). By turning on quantum spin-fluctuations, i.e., in the case of a mobile hole in a quantum antiferromagnet, the hole becomes a well-defined delocalized quasiparticle with the band minimum at $(\pi/2, \pi/2)$ and a bandwidth of the order of the antiferromagnetic spin-exchange coupling. In Ref. the string-excitations were extensively studied and it was found that they survive the turning on of quantum spin-fluctuations, i.e., they give rise to rather well-defined peaks in the hole spectral function at higher energies. In addition, as it is shown in this paper (see Fig. to be discussed later), they are responsible for the transfer of the quasiparticle weight from the low energy minimum at $(\pi/2, \pi/2)$ to the second and third string excitation as the $\Gamma$ point ($(0, 0)$) is approached and they are responsible for the observed vanishing of the quasiparticle weight near the $\Gamma$ point.

Next, in this paper, we will argue that the recently published results of the high resolution ARPES study or Ref. on the insulating cuprate Ga$_2$CuO$_2$Cl$_2$ provide strong evidence for the existence of these string-excitations. Furthermore, they yield their energy-momentum dispersion in agreement with the predictions made starting from the $t-J$ model. More generally these ARPES studies illuminate the role of string excitations in lightly doped quantum antiferromagnets and validate the theoretical framework which predicted them.

In order to make our arguments more convincing we will use the simpler $t-J$ model using the widely ac-
cepted values of the parameters $J/t = 0.3$ and $t = 0.4eV$ [12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22]. While, as we discussed there is a need to introduce next-nearest-neighbor hopping terms in order to reproduce the features of the quasiparticle band near $(\pi, 0)$, we will restrict our studies along the $(0, 0)$ to $(\pi, \pi)$ cut where these terms do not have a significant effect. Therefore, we will use the pure $t - J$ model with no free parameters, because the elegant aspects of the phenomenon that we try to convey can be described more clearly.

In Fig. 1 the spectral function of the $t - J$ model is presented for $J/t = 0.3$ along the $(0, 0) \rightarrow (\pi/2, \pi/2)$ calculated with the same approach as in Ref. 14. There is the main quasiparticle peak labeled I at low frequencies and at least two more visible peaks labeled II and III at higher frequencies. These peaks correspond to higher energy eigenstates of the simple 2D quantum "yo-yo" problem (a particle in a linearly rising potential) with the additional complication due to the fact that there is the quantum spin exchange term and the physics of this will be discussed later in this paper. One of the important aspects of the graph is the transfer of the spectral weight from the lowest energy peak (peak I) to the higher energy peak as the momentum changes from $(\pi/2, \pi/2)$ to $(0, 0)$. The physical explanation for the transfer of weight will be also given below after we make our case by comparing with the experiment. The second important aspect of the graph is that the spectral weight of the lowest energy peak nearly vanishes at the $\Gamma$ point of the Brillouin zone.

In Fig. 2 and Fig. 3 a comparison is made between the results of high resolution ARPES [22] as have been presented in Fig. 1 and Fig. 2 of Ref. 23. The theoretical results have been further broadened with a Gaussian broadening function, namely $A_\eta(k, \omega) = \int A(k, \omega')G(\omega - \omega')d\omega'$, where $G(\omega - \omega') = \exp(-((\omega - \omega')^2/\sigma^2)$, using $\sigma = 0.125eV$. Very similar results have been obtained if we use a value of $\eta = 0.125eV$ in the initial propagator (i.e., Lorentzian broadening) when we solve the Dyson’s equation. The same amount of broadening is also necessary to broaden the theoretical sharp quasiparticle peak so that its line-width is the same as the experimental one. This amount of broadening is very close to that used in Ref. 14 to compare the ARPES peak to the quasiparticle peak given by the $t - J$ model and its extensions. Notice, in Fig. 2 the transfer of weight from the lowest energy peak (most prominent at $(\pi/2, \pi/2)$) to another higher energy peak which forms as the momentum $(0, 0) \rightarrow (\pi/2, \pi/2)$. This seems to be the case in the most accurate ARPES data available from the insulator [22] and it becomes clearer in the following figure.

In Fig. 4 we compare the experimentally obtained intensity plot (top) to that obtained from the $t - J$ model.
FIG. 3: Comparison of the experimentally observed intensity plot reported in Fig. 2 of Ref. 23 (top) with that obtained from the $t-J$ model (bottom). The vertical energy scale in the theoretical curve (bottom) is similar to the experimental scale (top), i.e., about 1.5 eV. Notice the intense peaks at $(\pi/2, \pi/2)$ and near $(0, 0)$ in both theoretical and experimental intensity plots. At momentum $(0, 0)$ the spectral weight has been transferred to higher energy “string” states (II and III) as also seen in Fig. 1 and Fig. 2. This gradual transfer manifests itself as a more luminous path connecting the bright peaks at $(\pi/2, \pi/2)$ and $(0, 0)$.

for the same parameter values as those of Fig. 1 and the broadening procedure discussed above. Notice again that the gradual transfer of the spectral weight from the lowest energy peak to the higher energy peaks (mainly to the peaks labeled II and III in Fig. 1) appears as an “anomalous” high energy dispersion due to broadening and limited resolution. In other words, what appears to be a high energy dispersive curve is the dispersion of the center of “gravity” of the peaks II and III as they become more and more luminous as the value of momentum approaches $(0, 0)$.

Most recently in a different ARPES study an anomalous dispersion and a second energy scale at around 0.8 eV was reported[24]. This energy scale appears to be the center of “gravity” of the string excitation peaks II and III (measured from the lowest energy state at $(\pi/2, \pi/2)$) in our calculation, as can be seen by comparing our Fig. 1 with Fig. 2 of Ref. 24. Notice that, assuming that these features of the hole-band do not significantly change by doping, when the lowest energy quasiparticle states, which correspond to the lowest energy string states in the neighborhood of $(\pi/2, \pi/2)$, are occupied the higher lying string excitations will be probed by ARPES. The color-coded intensity plot of Fig. 3 excluding the bright spots around $(\pi/2, \pi/2)$ (because at sufficient amount of doping the states around $(\pi/2, \pi/2)$ should be inside the Fermi sea and the bright spots should move outside the Fermi surface), agrees reasonably well with the experimental intensity plots reported in Fig. 1 of Ref. 24. As can be clearly seen from these figures and the previous discussion, the process of spectral weight transfer to the higher string states is masked by low intensity and broadening and shows up as an “anomalous” dispersion with the center of the anomaly close to $(\pi/4, \pi/4)$ as in Fig. 1 of Ref. 24. It is surprising and perhaps revealing that these features persist all the way up to the overdoped regime. Therefore, it appears that the spin correlations should be strongly antiferromagnetic even in the overdoped cuprates.

We can give a qualitative picture of the origin of the spectral function peaks that correspond to the string excitations and a qualitative explanation of the spectral weight shift. Let us first discuss the single hole motion in a classical antiferromagnet, the so-called $t-J_z$ model. In this case as the hole moves away from its “birth” site, it displaces spins and, thus, it feels a potential which, as a function of the length of the hole path from its “birth” site, is linear with slope equal to
Therefore, in this limit the hole is almost localized and, for relatively large values of $t/J_z$, a quasi-continuum picture could be used to qualitatively describe the hole motion, where the energy levels are given by the form $E_n/t = \epsilon_n + a_n(J_z/t)^{2/3}$ and the corresponding wavefunctions are the Airy functions. Once the Heisenberg spin-exchange term $J_{zz}/2(s_i^+ s_j^- + s_i^- s_j^+)$ is turned on, two “string” states of overturned spins with the “birth” site at the beginning of each string and the hole at the end, which only differ by just two spins at the beginning of the string, can have significant overlap through this Heisenberg spin-exchange. This non-zero overlap can give favorable (lowering) contribution to the hole kinetic energy can take advantage from the overlap between two related strings is $e^{ikR} = -1$. Since, as we already mentioned, $R$ is the vectorial displacement of the hole after two consecutive nearest-neighbor hops, we find that the hole band must have minima at $(\pm \pi/2, \pm \pi/2)$ which is almost the case [4, 12]. We are now ready to discuss the question of why there is transfer of spectral weight to higher string-excitations as we approach the Π point. As this point is approached the kinetic energy lowering from the constructive interference of strings differing by a segment of two overturned spins can not be achieved through the phase factor associated with the translation operator (Bloch’s phase factor) because $k \to 0$. However, the desired phase coherence can be achieved by forming quasiparticle states in which the various string states are not included with amplitudes having the same phase but with an appropriate phase difference so that the kinetic energy can take advantage from the overlap between two such string states. Therefore, although $k \to (0,0)$ the quasiparticle state has nodes and, hence, it should overlap more with higher string excitations.

A rather simplified physical picture of a mobile hole in a quantum antiferromagnet may be given. The hole becomes a well-defined quasiparticle dressed with a cloud of strings of overturned spins which the quasiparticle carries with it. The hole in this cloud of strings or “string-bag” has internal excitations, which, as we argued, have been possibly observed in the high resolution ARPES studies [23, 24]. We have shown that the existence of such “internal” excitations of the “spin-polaron” are responsible for the vanishing of the quasiparticle from the lowest string state at the Π point and for the transfer of spectral weight to higher energy string excitations. In addition, they are responsible for the recently reported high energy anomalous dispersion in ARPES studies [23, 24].

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