Sharp Photoemission Spectra in the Quantum Antiferromagnet

S Sorella

INFM, International School for Advanced Study, Via Beirut 4, 34013 Trieste, Italy
Instituto de Ciencia de Materiales, Cantoblanco, 28049, Madrid, Spain

(November 12, 2021)

Abstract

The low energy photoemission spectra in quantum antiferromagnets are studied by using several approximation-free calculations and rigorous theorems. The important and measurable property found is that the hole eigenstates with momenta differing by the antiferromagnetic wavevector $Q$ are equivalent and degenerate in energy. However the corresponding eigenstates differs by the presence or the absence of a well defined quasiparticle corresponding to a singular -zero energy- magnon, carrying spin one and momentum $Q$. This difference between the two eigenstates affects dramatically the spectral weight as a function of the scattered momentum, since a sharp effect at the surface of the magnetic Brillouin zone is predicted, in apparent agreement with recent experimental data.
I. INTRODUCTION

Soon after the discovery of high-$T_c$ materials it was proposed that, this kind of interesting phenomenon, could be explained by the strong antiferromagnetic fluctuations characterizing the phase at small hole doping. The fact that in this regime the materials are close to a Mott-Hubbard transition have stimulated an intense scientific activity on the study of simple one band models, like the Hubbard model and the $t-J$ model, whose apparent simplicity is very attractive. However these models represent a still unsolved many-body problem in condensed matter physics, as it is still questioned whether they can have a superconducting ground state in two spatial dimensions.

The so called $t$-$J$ model is defined by the following hamiltonian:

$$H = -t \sum_{<i,j>,\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + h.c.) + J \sum_{<i,j>} (S_i \cdot S_j - \frac{1}{4} n_i n_j). \tag{1}$$

where the constraint of no double occupancy is understood. Here $c^\dagger_i (c_i)$ creates (annihilates) an electron at site $i$, $n_i = \sum_\sigma n_{i\sigma}$ is the corresponding density operator with $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$, the symbol $<i,j>$ means summation over nearest neighbors, $J$ is the super-exchange coupling and finally the spin density operator $S_i$ is defined by the Pauli matrices $\vec{\sigma}$: $S_i = \sum_{\sigma,\sigma'} c^\dagger_{i,\sigma} \frac{\vec{\sigma}_{\sigma,\sigma'}}{2} c_{i,\sigma'}$. Hereafter periodic boundary conditions are assumed on a lattice containing $L$ sites with $N_h$ holes ($L - N_h$ electrons). In these paper I will mainly focus on the property of a single hole $N_h = 1$, which was a subject of a vast literature starting from Nagaoka and Brinkmann and Rice in the early seventies. This problem is also important because the property of a single hole in a quantum antiferromagnet are experimentally accessible by angle resolved photoemission experiments that quite recently [1,2] have reached an high level of resolution and reproducibility especially in two dimensions. In fact, in absence of hole doping, it is widely accepted that the Copper-oxide planes are well described by an effective Heisenberg model (the term proportional to $J$ in [1]) with long range antiferromagnetic order in two dimensions [3]. When an electron is photoemitted, a single hole is free to propagate in the Copper-Oxide plane, by hopping from Copper site to Copper site with matrix elements...
described by the $t$ term in Eq. (1). It is reasonable to assume that interaction with the $p$ Oxygen bands and other effects cannot lead to a qualitative change of the model provided the Coulomb repulsion remains large to forbid double occupied sites and properly define the position of the hole in the lattice. In fact by taking the large $U$ limit of the Hubbard model, the lower Hubbard band is correctly described by the $t-J$ model, which represents therefore a realistic model for the interpretation of photoemission experiments at low energies.

One of the most important property is to understand whether a single hole can propagate as a free particle as in a conventional band insulator. In this case if an electron is extracted from the lower band it will remains for infinite time with the given hole momentum $k$. Within the quasiparticle picture it is clear that interaction can provide a finite lifetime, but since in an insulator all the possible states in the lower band are occupied there is no phase space for decaying processes at least for the lowest possible excitations. As in the Landau theory for Fermi liquids it is then possible to define the so called quasiparticle weight $Z_p$, which measures the distance between the many body state $|p\rangle$ of a single hole and the corresponding ground state of the insulator $|H\rangle$ in which a hole has been created with momentum $p$ and spin $\sigma$, $c_{p,\sigma}|H\rangle$. The quasiparticle weight is then given by:

$$Z_p = |<p|c_{p,\sigma}|H\rangle|^2$$

For a band insulator with no interaction $Z_p$ is one by definition, whereas if a quasiparticle picture is well defined $Z_p$ remains finite in the infinite volume limit. A key question is to understand whether in two spatial dimension a quasiparticle theory can be defined for an insulator or if this quantity vanishes with a power law as in one dimension [4]. In particular in an antiferromagnet it is crucial to understand if the scattering with the underlying low energy modes—the spin wave excitations—can lead to some anomalous effect.

By the Lehman decomposition of the one particle Greens function $G_p(\omega)$ the finiteness of the quasiparticle weight $Z_p$ determines a $\delta$—function in the spectral weight $A(\omega < 0) = -\frac{1}{\pi}G_p(\omega)$, which, as mentioned, is experimentally accessible by ARPES. However it is difficult to distinguish, in an experiment, which is biased by the resolution of the
electronic device, if a true $\delta$ function exists or if the spectral weight is completely incoherent, i.e. without $\delta$ function contributions. This $\delta-$ function weight $Z_p$ occurs at an energy $E_p$, which represents, within the quasiparticle picture, the lowest one hole energy with given momentum $p$, and $E_p$ properly describes the energy dispersion of the hole.

In two spatial dimensions there is no exact solution of the “one hole problem” but there is a general believe that the basic dynamical properties of a single hole in a quantum antiferromagnet are well described in the paper by Kane Lee and Read (KLR) \[5\]. In this work the problem is solved using two main approximations: a large spin limit and a self consistent Born approximation to sum the relevant diagrams contributing to the Greens function, accounting for the scattering of the hole with the spin-waves. Within these approximations i) the quasiparticle weight is finite, ii) the minimum possible energy $E_p$ is generally at momentum $p = (\frac{\pi}{2}, \frac{\pi}{2})$ and finally, as a general property coming from the long range antiferromagnetic order, iii) momenta differing by the wavevector $Q = (\pi, \pi)$ are equivalent both for the energy and for the quasiparticle weight:

$$Z_p = Z_{p+Q}$$
$$E_p = E_{p+Q}. \quad (3)$$

In the original KLR paper there was some speculation that $Z_p$ could vanish away from the bottom of the band even within their approximations. However it was shown later \[6,7\] that $Z_p$ is strictly finite for all possible momenta in the Brillouin zone as long as $J > 0$.

An accurate determination of the single hole dispersion was recently determined by Quantum Monte Carlo and is essentially in agreement with the KLR result. The minimum of the band at $p = (\frac{\pi}{2}, \frac{\pi}{2})$ is also confirmed experimentally. \[1\] For the quasiparticle weight Quantum Monte Carlo is not accurate enough and, quite recently, the accuracy of the KLR theory has been questioned since numerical data obtained with Lanczos exact diagonalization up to 26 sites clearly showed that $Z_{p+Q} << Z_p$ at least for $p \sim 0$. \[8\]

I will show in this paper (and prove for $J = 2t$) that while the spectrum satisfies \( \delta \) (rigorously shown in App. \( \text{VIII} \) using a variational ansaz), the quasiparticle weight $Z_p \neq Z_{p+Q}$. 


This effect induces a kind of Fermi volume discontinuity which is consistent with recent experiments by Wells. In this work it was pointed out that the photoemission experiments of insulating antiferromagnetic materials look similar to the corresponding metallic ones. This simple effect is instead a direct consequence of a singular magnon excitation present in a quantum antiferromagnet which cost zero energy and change the spin by one and the momentum by $Q$. In essence this strange and measurable effect is intimately related to the non commutativity of the order parameter $\mathbf{m}$ with the total spin $\mathbf{S}^2$. In any mean field theory one usually selects a direction of the order parameter and in this way the spin is no longer defined for the approximate ground state. In an experiments however the variation of the total spin is measured since the outcoming electrons have a definite spin. An approach which is capable to work in a basis with definite spin $\mathbf{S}^2$ and order parameter $\mathbf{m}^2$ allows to deal correctly with the excitations and to determine the sharpness of the photoemission spectra in a quantum antiferromagnet.

II. FORMALISM

I consider the $t - J$ Hamiltonian (1) and follow the formalism recently proposed by Angelucci et al. The basic advantage of this approach is the possibility to simplify the local constraint of no doubly occupied sites by extending the hamiltonian to an enlarged space, where the physical subspace, satisfying the constraint, is obtained when the eigenvalue of a spin-operator $\mathbf{L}$ is maximum. In this representation the $t - J$ Hamiltonian matrix reads

$$H = E_0 + \sum_{R, \tau \mu} \left[ t (f_{R+\tau \mu}^\dagger f_R + \frac{J}{4} (1 - n_R - n_{R+\tau \mu}) \right] \chi_{R,R+\tau \mu}. \quad (4)$$

where $f_R^\dagger$ and $f_R$ are canonical spinless fermion operators creating or annihilating a hole at site $R$ and commuting with the corresponding spin operators $\mathbf{S}_R$. Moreover $n_R = f_R^\dagger f_R$ is the hole number at the site $R$, $N_h = \sum_R n_R$ being the total number of holes, and the operator

$$\chi_{R,R'} = 2\mathbf{S}_R \mathbf{S}_{R'} + \frac{1}{2} \quad (5)$$
interchanges two $S = 1/2$-spins at sites $R$ and $R'$. Hereafter periodic boundary conditions over a finite hyper-cubic box with linear size $l$ and number of sites $L = l^d$ is assumed. The constant shift of the energies $E_0 = Jd/2(2N_h - L)$, which represents the classical contribution of an antiferromagnetic Néel state, is also omitted.

The hamiltonian (4) is naturally defined in a space where there is a single spin for each site and the hole can be created over each spin site by $f^\dagger$. However the spin value at the position of the holes is clearly unphysical because in the physical Hilbert space the hole does not carry spin. As anticipated this difficulty can be easily solved because the hamiltonian leaves invariant the physical subspace of states where the spins over the sites occupied by the holes are all frozen to $1/2$ (or $-1/2$). In fact the following pseudo-spin operator, measuring the total spin at the positions of the holes, and satisfying the algebra of the angular momentum

$$\vec{L} = \sum_R n_R \vec{S}_R,$$

commutes with the Hamiltonian (4) and the invariant subspace with maximum spin $L = L_z = N_h/2$, coincides with the physical Hilbert space of the $t - J$ model, where the two models have the same matrix elements, i.e. they identically coincide.

Analogously the physical total spin has to be measured where there are no holes and within the present formalism it is defined by:

$$\vec{S} = \sum_R (1 - n_R) \vec{S}_R,$$

Even this operator commutes with the hamiltonian and obviously with the pseudo-spin $\vec{L}$. In the following sections the total spin

$$\vec{S}_{\text{tot}} = \vec{S} + \vec{L}$$

will be introduced too.

Any eigenstate $|\psi\rangle$ of the hamiltonian can be labeled by six quantum numbers:

- The number of holes $N_h$
• The value of the physical spin $S$ and its component on the z-axis $S_z$
• The value of the pseudo-spin $\bar{L}$ and its component on the z-axis $L_z$
• The total lattice momentum $p$ of the state.

and the physical sector is obtained when $\bar{L} = L_z = \frac{N}{2}$. Correlation functions are expectation value of operators $\hat{O}$ over these eigenstates $\langle \psi | \hat{O} | \psi \rangle$. If such an operator commutes with the total spin $\vec{S}$ or the pseudo-spin $\vec{L}$ -as, say, the hamiltonian- the corresponding expectation value does not depend on the spin component on the z-axis $S_z$ or $L_z$. In particular all the eigenstates differing by the quantum number $L_z$ or $S_z$ are degenerate.

At the end of this section we remind that a state $|\psi_p\rangle$ with definite lattice momentum $p$ is an eigenstate of the translation operator $T_R$, such that $T_R|\psi_p\rangle = e^{-ipR}|\psi_p\rangle$. The operator $T_R$ is the translation operator that brings the origin $O$ to the lattice point $R$. It is formally defined by the following relations valid for any $R$ and $R'$:

$$T_R f_R T_{-R} = f_{R+R'}$$
$$T_R \vec{S}_R T_{-R} = \vec{S}_{R+R'}$$

The lattice momentum $p$ is defined in the Brillouin zone (BZ) with each component $|p_i| \leq \pi$ (the lattice constant is one). An important region contained in the previous one is the magnetic Brillouin zone (BZ') defined as the locus of points such that $\gamma_p \geq 0$ where $\gamma_p = \frac{1}{2d} \sum_{\mu} e^{ip_{\mu} R_{\mu}}$.

### III. TOWER OF STATES IN A QUANTUM ANTIFERROMAGNET

In a quantum antiferromagnet the most important quantities for the correct description of the low energy physics are the order parameter $\vec{m}$ and the total spin $\vec{S}$, that, within our formalism, read:

$$\vec{m} = \frac{1}{L} \sum_{R} e^{iQR} \vec{S}_R (1 - n_R)$$
$$\vec{S} = \sum_{R} \vec{S}_R (1 - n_R)$$

(10)
where $Q$ is the antiferromagnetic wavevector $Q = (\pi, \pi, \cdots)$

The commutation rules of these two operators are well known [9]:

\[
\begin{align*}
[S_j, m_k] &= i\epsilon_{j,k,l}m_l \\
[S_j, S_k] &= i\epsilon_{j,k,l}S_l \\
[m_j, m_k] &= i\frac{L^2}{2}\epsilon_{j,k,l}S_l
\end{align*}
\]  

In particular using the above relations it is easy to obtain the commutation of $m^+ = m_x + im_y$ or $m^- = m_x - im_y$ and $m_z$ with the total spin $\vec{S}^2$:

\[
\begin{align*}
\left[\vec{S}^2, m^+\right] &= -2m_zS^+ + 2m^+(1 + S_z) \\
\left[\vec{S}^2, m^-\right] &= 2m_zS^- + 2m^-(1 - S_z) \\
\left[\vec{S}^2, m_z\right] &= m^-S^+ - m^+S^- + 2m_z
\end{align*}
\]  

The operator $m^2$ commutes with $\vec{S}^2$ and $S_z$. In the following it will be assumed that $\vec{m}^2$ also commutes with the hamiltonian since if long range order sets in $\vec{m}^2$ becomes a macroscopic classical variable in the infinite volume limit. [10] Then we may classify the eigenstates in terms of the four quantum numbers $\vec{S}^2$, $S_z$, $\vec{m}^2$ and the total lattice momentum of the eigenstate.

Suppose that an eigenstate $|S, m^2, \vec{p}\rangle$ is given with total momentum $\vec{p}$, definite spin $S$ and maximum azimuthal spin $S_z = S$, (all the other $S_z$ component can be easily obtained by a repeated application of the total spin lowering operator $S^-$), it will be shown in the following that the state $m^+|S, m^2, \vec{p}\rangle$ has spin $S + 1$, $S_z = S + 1$, the same order parameter $\vec{m}^2$ but momentum $\vec{p} + Q$.

The change of momentum is easily understood since $T_R\vec{m}T_{-R} = e^{iQR}\vec{m}$, yielding $T_Rm^+|S, m^2, \vec{p}\rangle = e^{i(p+Q)R}m^+|S, m^2, \vec{p}\rangle$, i.e. a state with momentum $\vec{p} + Q$. On the other hand, by hypothesis:

\[
\vec{S}^2|S, m^2, \vec{p}\rangle = S(S + 1)|S, m, \vec{p}\rangle
\]
whereas by applying (12):

\[
\vec{S}^2 m^+ |S, m^2, p> = (m^+ \vec{S}^2 + [\vec{S}^2, m^+]) |S, m^2, p> = (S + 1)(S + 2)m^+ |S, m^2, p> ,
\]
i.e. \(m^+ |S, m^2, p>\) is a state with definite spin equal to \(S + 1\). Analogously \(S_z\) is defined since, by \([S_z, m^+] = m^+\), it follows \(S_z m^+ |S, m^2, p> = (S + 1)m^+ |S, m^2, p>\). Finally \(\vec{m}^2\) does not change by applying \(m^+\) to the state \(|S, m^2, p>\) as \([\vec{m}^2, m^+] = 0\).

By the simple assumption that \(m^2\) commutes with the hamiltonian for \(L \to \infty\), it has been derived that all the different spin sectors are degenerate and the momentum is defined modulo \(Q\). In a finite system this degeneracy is slightly removed and in fact the energy spectrum as a function of the spin behaves as a free quantum rotator spectrum determined by the value of its static susceptibility \(\chi_{ST}\) \cite{11,12}:

\[
E(S) = E_0 + \frac{S(S + 1)}{2L \chi_{ST}} + o\left(\frac{1}{L}\right).
\]
Instead by spin-wave theory the magnon excitations are characterized by much larger energy costs \(\sim \frac{1}{L}\). It seems therefore exact at least at low enough energies that the tower of states with different spin can be considered degenerate for \(L \to \infty\), when \(\vec{m}^2\) becomes classical. In a bipartite lattice without holes the spin is integer and the lowest eigenstates with \(S = n\) can be obtained by applying \(n\) times the operator \(m^+\) to the singlet spectrum of eigenstates \(|S = 0, m^2, p>\):

\[
|S + n, m^2, p + nQ > \propto (m^+)^n |S, m^2, p> \tag{13}
\]
In particular, from \(2Q = 0\) modulo \(2\pi\), odd integer spin have the lowest energy state with momentum \(Q\), whereas even spin have vanishing momentum (referenced to the singlet momentum which is 0 or \(Q\) according to the parity of \(L\) respectively).

In presence of a single hole or an odd number of holes the spin is half odd integer (for half odd integer spin \(s\)) and the minimum one is \(S = \frac{1}{2}\). Consequently the eigenstate with minimum spin, generator of all the tower of states in (13), has non vanishing spin \(S = \frac{1}{2}\). In this case a further operator is relevant to generate all the manifold of degenerate states.
since by applying $(\vec{m} \cdot \vec{S})$ to an element $|S,m^2,p> \text{ of the tower (13)}$ one gets a different state with the same spin (due to the rotationally invariant expression $(\vec{m} \cdot \vec{S})$, commuting with the total spin) but momentum $p + Q$:

$$|S,m^2,p + Q> \propto (\vec{m} \cdot \vec{S})|S,m^2,p> \text{.}$$

(14)

In fact, by using (11), the operator $(\vec{m} \cdot \vec{S})$ commutes with $m^+$ and obviously annihilates any singlet state. Hence the expression (14) defines non vanishing states only in the half-odd integer spin case where the lowest spin state of the tower has $S = \frac{1}{2}$. The new relation (14) cannot be iterated as the previous one (13), because the square of the operator $(\vec{S} \cdot \vec{m})$ when applied to the generator state $|S = \frac{1}{2}, m^2,p>$ behaves as a constant equal to $\frac{(\vec{m})^2}{4} + o(\frac{1}{L})$. In fact $(\vec{m} \cdot \vec{S})^2 = \frac{1}{2} \left[ \sum_{i,j} m^i m^j (S^i S^j + S^j S^i) \right] + \frac{(\vec{S})^2}{2L^2} \text{ and } S^i S^j + S^j S^i = \frac{1}{2} \delta_{i,j} \text{ on a spin-}\frac{1}{2} \text{ state.}

The final diagram of the tower of degenerate states (or almost degenerate states at finite size) are shown in the following diagram:

$$|S + 1, m^2,p + Q> \Rightarrow |S + 1, m^2,p> \text{ (}\vec{S} \cdot \vec{m}) \text{ (15)}$$

$$\uparrow m^+ \quad \uparrow m^+$$

$$|S, m^2,p> \Rightarrow |S, m^2,p + Q> \text{ (}\vec{S} \cdot \vec{m})$$

$$|\frac{1}{2}, m^2,p> \Rightarrow |\frac{1}{2}, m^2,p + Q>$$

We expect therefore that for odd number of holes and fixed spin (and maximum azimuthal spin) all the spectrum is characterized by couples of eigenstates with momenta $p$ and $p + Q$ related by the approximate expression (13).

Indeed for the single hole case it can be rigorously shown (see App. VIII) that the lowest eigenstates with momenta $p$ and $p + Q$ differ in energy by terms less than $\sim \frac{1}{L}$. Moreover the relation (14) between such a couple of states is exact within the assumption that in any subspace with given spin and momentum the gap to the first excited state scales as $\sim \frac{1}{L}$ (
one has to excite at least one \( k \neq 0, Q \) magnon in this case), i.e. much larger than the energy accuracy \( \sim \frac{1}{L} \) of the state (14). In the next section (VI) it will be shown that Eq. (14) is indeed consistent with the exact solution obtained for momenta \( p = 0 \) and \( p = Q \) at the supersymmetric point \( J = 2t \). [13]

The general character of the spectrum in a quantum antiferromagnet does not depend upon doping if long range magnetic order exists with finite momentum \( Q \). However the basic relation (14) is expected to be only approximate at finite doping, because charge excitations with energy cost \( \sim \frac{1}{L} \) are known to exist (invalidating the assumption of a gap scaling as \( \frac{1}{L} \)), as it is also clear from the weak coupling theory in the Hubbard model.

It is a luck that for a single hole, charge excitations are forbidden by the requirement of fixed total momentum, and relation (14) is asymptotically exact for the lowest possible energy in each subspace with given momentum. Lowest energy eigenstates with momenta differing by \( Q \) are characterized by quite different eigenfunctions satisfying relation (14). In two dimension momenta \( p \) and \( p + Q \) are equivalent by spatial symmetry on the surface of the magnetic Brillouin zone. Thus one expects some discontinuity or at least some singularity as the momentum of the hole crosses the magnetic Brillouin zone. This should hold at least for physical quantities, like the quasiparticle weight (see Sec. V), explicitly depending on the momentum dependent lowest energy state \( |\psi_p> \).

**IV. EXACT INTEGRATION OF THE SINGLE HOLE CHARGE**

The hamiltonian (4) is translation invariant and the most general one-hole state with total lattice momentum \(-p\) (hole momentum \( p \)) can be written:

\[
|\psi_p> = \frac{1}{\sqrt{L}} \sum_R e^{ipR} f_R^\dagger T_R |S> \tag{16}
\]

where \( |S> \) is a pure spin state without holes, i.e. \( f_i |S> = 0 \).

The state \( |\psi_p> \) in (16) represents the most general one-hole state \((N_h = 1)\) with given hole momentum \( p \). The action of any translation invariant operator \( \hat{O} \) over the state \( |\psi_p> \)
does not change the momentum of the resulting state $\hat{O}|\psi_p >$ and is therefore equivalent to the action of an effective spin operator $O^{\text{eff}}$ acting on $|S >$, defined by:

$$\hat{O}|\psi_p > = \frac{1}{\sqrt{L}} \sum_R e^{ipR} f^\dagger_R T_R O^{\text{eff}} |S >$$

(17)

For instance consider the kinetic term of the hamiltonian (4) along one particular direction $\mu$:

$$K_\mu = \sum_{R'} f^\dagger_{R+\tau_\mu} f_{R'} \chi_{R',R'+\tau_\mu}.$$  

(18)

Using that the state $|S >$ and all the translated ones $T_R|S >$ contain no holes $f_{R'} f^\dagger_R T_R|S > = \delta_{R,R'} T_R|S >$, $K_\mu|\psi_p >$ is easily computed:

$$K_\mu|\psi_p > = \frac{1}{\sqrt{L}} \sum_R f^\dagger_{R+\tau_\mu} \chi_{R,R+\tau_\mu} e^{ipR} T_R|S >$$

Then changing $R + \tau_\mu \rightarrow R$ in the dummy summation and using the translation operator rule $T_{R-\tau_\mu} = T_R T_{-\tau_\mu}$:

$$K_\mu|\psi_p > = \frac{1}{\sqrt{L}} \sum_R f^\dagger_{R} \chi_{R-\tau_\mu,R} e^{ip(R-\tau_\mu)} T_{R-\tau_\mu}|S > = \frac{1}{\sqrt{L}} \sum_R f^\dagger_{R} e^{ipR} T_R \chi_{O,-\tau_\mu} e^{-ip\tau_\mu} T_{-\tau_\mu}|S >$$

where in the latter equality $T_{-R} \chi_{R-\tau_\mu,R} T_R = \chi_{-\tau_\mu,O}$ comes directly from (9). Finally, consistent with Eq. (17), it follows that:

$$K^{\text{eff}}_\mu = \chi_{O,-\tau_\mu} e^{-ip\tau_\mu} T_{-\tau_\mu}$$

(19)

Analogously it is a simple algebra to show that the effective spin hamiltonian reads:

$$H^{\text{eff}}_p = \sum_{\tau_\mu} \chi_{O,\tau_\mu} (te^{ip\tau_\mu} T_{\tau_\mu} - J/2) + H_{SW}$$

(20)

where $H_{SW}$ is the translation invariant Heisenberg hamiltonian

$$H_{SW} = -\frac{J}{4} \sum_{R,\tau_\mu} \chi_{R,R+\tau_\mu}.$$  

The total spin $\vec{S}_{tot} = \sum_R \vec{S}_R$ of the effective spin hamiltonian remains unchanged with respect to the old definition (8) and measures the total spin in the whole lattice including the origin.
site \( O \), whereas the pseudo-spin \( \vec{L} \), the physical spin \( \vec{S} \) and the staggered magnetization \( \vec{m} \) turn in:

\[
\begin{align*}
\vec{L}^{\text{eff}} & \to \vec{S}_O \\
\vec{S}^{\text{eff}} & \to \vec{S}_O^{\text{tot}} - \vec{S}_O \\
\vec{m}^{\text{eff}} & \to \vec{m} - \frac{\vec{S}_O}{L}
\end{align*}
\]  

(21)

(22)

The pseudo-spin and the physical spin operators commute with the effective spin hamiltonian (20), as it is easy to check. Thus there is a one to one correspondence of any eigenstate of the effective spin hamiltonian with any single-hole eigenstate with given momentum of the extended hamiltonian (4). The identification of the true eigenstates of the \( t-J \) model is in this case trivial, because the total pseudo-spin \( L \) is fixed to \( \frac{1}{2} \) and the extended hamiltonian does not have eigenstates with unphysical pseudo-spin \( L \neq \frac{N_h}{2} \). This property is valid only for the one hole case as it is discussed in [8].

In the following it will be established a correspondence between the eigenstates of the well known Heisenberg hamiltonian and the eigenstates of \( H_p^{\text{eff}} \). To this purpose it is convenient to use the total spin \( S^{\text{tot}} \) and its z-component \( S^{\text{tot}}_z \) as good quantum numbers for the eigenstates \( |S^{\text{tot}}, S^{\text{tot}}_z > \) of (24). The total spin of the effective hamiltonian \( \vec{S}^{\text{tot}} = \vec{L}^{\text{eff}} + \vec{S}^{\text{eff}} \) corresponds to the sum of the physical spin with the pseudospin. It commutes with the hamiltonian but does not commute with each component of the pseudospin \( \vec{S}_O \).

In order to have a definite total spin \( S^{\text{tot}} \), each eigenstate with physical spin \( S \) (with all the degenerate \( 2S + 1 \) components) has to combine with the two values of the spin at the origin, yielding eigenstates, with total spin \( S^{\text{tot}} = S + \frac{1}{2} \) and with \( S^{\text{tot}} = S - \frac{1}{2} \), by the well known addition relations of angular momenta. After projecting each eigenstate \( |S^{\text{tot}}, S^{\text{tot}}_z > \) onto the ones with definite \( S^{\text{tot}}_O = \frac{1}{2} \), i.e \( \left< S_O \right| (\frac{1}{2} + S^{\text{tot}}_O)|S^{\text{tot}}, S^{\text{tot}}_z > \) the physical spin of the corresponding hole eigenstates (13) is \( |S^{\text{tot}} \pm 1/2 > \). The physical spin is thus univocally determined to be \( S = \frac{1}{2} \) in the singlet total spin \( S^{\text{tot}} = 0 \) subspace. It is possible to avoid any ambiguity by restricting all the following analysis to this subspace, which in turn is important for the analysis of photoemission experiments in stoechiometric compounds.
In fact these experiments determine the imaginary part of the Greens function, that, at half filling, reads:

\[ G(p, t) = -i < H | c_p^\dagger e^{-i(H - i\delta - E_0)t} c_p | H > \]  

, i.e. it is obtained by creating a hole over the singlet antiferromagnetic state \( |H> \). \cite{14}

Thus only the singlet subspace of the effective hamiltonian is relevant for the calculation of the Greens function in an antiferromagnetic insulator.

In the singlet subspace we can use the total spin \( S_{\text{tot}} \) to classify the spin of the elementary excitations, analogously to what was done in the 1D Heisenberg model where the spinons have been found to carry spin \( \frac{1}{2} \). \cite{15}

The hamiltonian (20) is exact, and the presence of the translation operator makes difficult to use standard approaches as for the simpler \( H_{SW} \). The recent ansatz \cite{9} proposed by Shraiman and Siggia corresponds to a variational semiclassical solution of the hamiltonian (20), yielding for example the Néel state for \( H_{SW} \). However in the one hole case the semiclassical solution cannot be controlled by the small parameter \( 1/s \), important to derive the spin-wave limit for the Heisenberg model. \cite{16}

V. QUASIPARTICLE WEIGHT, GREENS FUNCTION AND CURRENT OPERATORS

After the introduction of the effective spin hamiltonian (20) the Greens function (23) is easily expressed as an expectation value of a spin operator acting on the Heisenberg ground state \( |H> \).

The state \( |\psi_p> = c_{p,\sigma} |H> \) is of the form \( (16) \), if we choose \( |S> = |S_H> \) with:

\[ |S_H> = n_{\sigma,0} |H> . \]  

Due to the correspondence of eigenstates between \( H_p^{\text{eff}} \) and \( H \), we can expand \( |S> \) in terms of eigenstates of \( H_p^{\text{eff}} \) and easily check that the propagation of \( |S_H> \) with the effective
Hamiltonian, \( |S_H > = e^{-iH_{p}^{eff}t}|S_H > \), corresponds exactly to the propagation of \( \psi_p \) with the exact \( t-J \) Hamiltonian and the Greens function immediately follows:

\[
G(p,t) = -\frac{i}{2} <S_H|e^{-i(H_{p}^{eff} - i\delta)t}|S_H >
\]  

(25)

Using that \( |S_H > = \sqrt{2}n_{i,\sigma}|H > \), that the commutator \( [H_{p}^{eff},n_{\sigma,O}] \) vanishes and that \( G \) does not depend on \( \sigma \), we get, after Fourier transform \( G(p,\omega) = \int_0^\infty dt \ G(p,t) \ e^{i\omega t} \),

\[
G(p,\omega) = \frac{1}{2} <H|\frac{1}{\omega + i\delta - H_{p}^{eff}}|H > .
\]  

(26)

The factor \( \frac{1}{2} \) is usually omitted in the literature of strong coupling theories like the \( t-J \) model, probably for estetic reasons of normalizations. Here we are interested to the actual photoemission delta weight and we are not allowed to use misleading normalizations.

Once \( H_{p}^{eff} \) is diagonalized by eigenstates \( |i > \) with total vanishing spin \( \vec{S}_{tot} = \vec{S} + \vec{S}_O \) and energies \( E_i \) the Greens function is obtained by inserting this complete set of eigenstates in (26):

\[
G(p,\omega) = \frac{1}{2} \sum_i | <H|p >_i |^2 \frac{1}{\omega + i\delta - E_i}
\]  

(27)

A general relation satisfied by the Greens function of a single hole in an antiferromagnet directly follows from the property that the lowest eigenstate \( |p + Q > \) of \( H_{p+Q}^{eff} \) can be written in term of the eigenstate \( |p > \) of \( H_{p}^{eff} \) using relation (14) and (22) valid at low energy, i.e. \( |p + Q > i \propto (\vec{S}_{eff} \cdot \vec{m}_{eff})|p >_i = -(\vec{S}_O \cdot \vec{m}_{eff})|p >_i = -(\vec{S}_O \cdot \vec{m})|p >_i \) where in the latter equalities we have used that \( |p >_i \) are singlet states and we have neglected the \( O(\frac{1}{L}) \) difference between the physical staggered magnetization \( \vec{m}_{eff} \) (22) and the one acting over all the sites \( \vec{m} = \vec{m}_{eff} + \vec{S}_L \). A simple normalization is then possible using Eq. (51), and by neglecting \( O(\frac{1}{L}) \) contributions one obtains consistently:

\[
|p + Q >_i = \frac{2}{m} (\vec{S}_O \cdot \vec{m})|p >_i .
\]  

(28)

for the lowest energy state in each fixed momentum sector.
The imaginary part of the Greens function is experimentally accessible by angle resolved photoemission experiments (ARPES) and we will refer to it as the spectral function $A(\omega)$. In the imaginary part of (27) some of the $\delta$ function weights may remain finite for $L \to \infty$ and define the so called quasiparticle weight $Z_p$, which is usually a single peak located at the bottom of the finite size spectrum [17]. All the other part of the spectrum merge in a continuum of states for $L \to \infty$ leading to an incoherent spectral function.

Using (27) the quasiparticle weight is given by:

$$Z_p = \frac{1}{2} \langle | S \rangle_p^2$$

(29)

where $| S \rangle_p$ is the lowest energy singlet state of the hamiltonian $H_p^{eff}$. Notice that the quasiparticle weight in a strong coupling theory cannot exceed the value $\frac{1}{2}$ since it is obviously bounded by the value of the momentum distribution $n_p = \langle | c_p^\dagger c_p | H \rangle = \frac{1}{2}$. Notice that using (28) $Z_{p+Q}$ can be expressed in the following form:

$$Z_{p+Q} = \frac{2}{m^2} \langle | H | (\vec{m} \cdot \vec{S}_O) | S \rangle_p^2$$

(30)

This is an asymptotically exact relation for $L \to \infty$, as long as $m > 0$, i.e. within the assumption of long range magnetic order.

Another important quantity to study is the current operator, which is useful when we calculate the transport properties. On a discrete lattice, the current operator corresponding to a uniform field is defined by [18]:

$$J_\mu = \left[ i e t \sum_{R\sigma} c_{R\sigma}^{\dagger} c_{R+\tau_\mu \sigma} + \text{h.c.} \right]$$

(31)

In terms of spinless fermion hole operators $f_i$ and spin interchange ones $\chi_{i,j}$ the total current is given by:

$$J_\mu = \left[ i e t \sum_{R\sigma} f_{R\sigma} f_{R+\tau_\mu}^{\dagger} \chi_{R,R+\tau_\mu} + \text{h.c.} \right]$$

(32)

We note that $J_\mu = -ie(K_\mu - K^-_\mu)$ where $K_\mu$ is defined in [18], thus when applied to a state of the form (16) the effective current operator, acting only on a spin wavefunction, can be written as.
\[ J_{\mu}^{\text{eff}} = [iet\chi_{0,\tau_{\mu}} e^{ip\tau_{\mu}} T_{\tau_{\mu}} + \text{h.c.}] \] (33)

Following [19] the real part of the conductivity in a uniform field is characterized by a \( \delta \) function proportional to the hole kinetic energy per site and a paramagnetic contribution given by the Kubo formula:

\[
\sigma(\omega)_{\mu} = e^2 K_{\mu} + \Lambda_{\mu}(\omega)\frac{i}{i(\omega + i\delta)}
\] (34)

where \( K_{\mu} = t\chi_{0,\tau_{\mu}} e^{ip\tau_{\mu}} \) is the kinetic energy in the direction \( \mu \) and \( \Lambda \) is given by:

\[
\text{Im} \Lambda_{\mu}(\omega) = \sum_{j} |<p|J_{\mu}|p_j>|^2 \delta(\omega - \omega_j)
\] (35)

where the sum over \( j \) indicates the eigenstates with the same momentum \( p \) of the single hole ground state, \( \omega_j \) being the corresponding energy excitations referred to the ground state energy.

Of course a factor \( \frac{1}{L} \) have been dropped out in the previous expressions for the conductivity because there is only a single charge allowed to move. At small doping the conductivity will be proportional to the number of carriers times the conductivity of the single hole, i.e. will be finite in the thermodynamic limit.

VI. SOME EXACT EIGENSTATES FOR THE SUPERSYMMETRIC POINT

At the supersymmetric point for \( J = 2t \) the kinetic part proportional to \( t \) is exactly canceled by the magnetic bonds around the origin in (20). In fact any eigenstate \( |q> \) of the Heisenberg hamiltonian \( H_{SW} \) with total momentum \( q = p \) is an exact eigenstate of (20) with the same hole momentum \( p \) and energy \( E_p \). In fact by assumption \( H_{SW}|p> = E_p|p> \) and \( T_{\tau_{\mu}}|p> = e^{-ip\tau_{\mu}}|p> \), and immediately follows that:

\[
H_{\mu}^{\text{eff}}|p> = E_p|p> + t \sum_{\tau_{\mu}} \chi_{0,\tau_{\mu}}(e^{ip\tau_{\mu}} T_{\tau_{\mu}} - 1)|p> = E_p|p>
\] (36)

The collection of all possible one hole states with arbitrary hole momentum has clearly an Hilbert space dimension \( \sim L \) times the dimension of the Heisenberg model. Thus the
Heisenberg eigenstates with all possible momenta \( q \) are not a complete set for the one hole Hilbert space. It is remarkable however that for \( J = 2t \) a considerable fraction (\( \sim \frac{1}{2} \)) of all the eigenstates is exactly known and indeed coincide with the ones of \( H_{SW} \). I have verified numerically up to 26 site 2D-lattice that the lowest-energy one-hole eigenstates with momentum \( p = 0 \) or \( p = Q = (\pi, \pi) \) are of the previous type, i.e. particular eigenstates of the Heisenberg model. For \( p = 0 \) in any spatial dimension the singlet spin state \( |S> \) characterizing the single hole eigenstate \(|H>\) coincides with the true ground state of the Heisenberg Hamiltonian \(|H>\), the quasiparticle weight is exactly one and exhausts all the spectral weight, \( A_{p=0} = \frac{1}{2}\delta(\omega - E_{p=0}). \)

An interesting feature instead is when the momentum of the hole coincides with the antiferromagnetic wavevector \( Q = (\pi, \pi, \cdots) \). In this case the singlet state \( |S> \) characterizing the lowest possible one hole eigenstate with momentum \( Q \) can be obtained using the first excitation of the Heisenberg model, which has momentum \( Q \) and is a triplet:

\[
|H,\sigma> \quad \text{for} \quad \sigma = -1, 0, 1
\]

\[
|H,1> = \frac{1}{\sqrt{2}}S^+|H,0> \quad |H,-1> = \frac{1}{\sqrt{2}}S^-|H,0>
\]

with energy \( E_{p=0} + \frac{1}{L\chi_{ST}} + o(\frac{1}{L}) \), where \( \chi_{ST} \) is the static spin susceptibility of the Heisenberg model. The above states can be combined with the operator \( \tilde{S}_O \) which commutes with the Hamiltonian, leading to nine different spin eigenstates \( S_O^j|H_\sigma> \) for \( j,\sigma = 1, 2, 3 \) with the same energy and with spin components on the \( S = 0, 1, 2 \) subspaces. By a proper linear combination of these states it is then possible to select an exact singlet eigenstate in the following way:

\[
|S>_{Q} = \alpha \left( S_O^+S^-|H,0> - S_O^-S^+|H,0> + 2S_O^z|H,0> \right)
\]

where the normalization constant \( \alpha \) is easily computed, yielding:

\[
\alpha^2 \rightarrow \frac{1}{3} + O(\frac{1}{L})
\]

After a little algebra, using that both \(|H>\) and \(|H,\sigma>\) have definite momenta, the
overlap of this state with the Heisenberg ground state is:

\[ < H|S >_Q = 6\alpha < H|m_z^Q|H,0 > \]

leading, by means of the Schwartz inequality, to:

\[ Z_Q = \frac{1}{2} < H|S >_Q^2 \leq 18\alpha^2 < H|(m_z^Q)^2|H,0 > = 2m^2 \tag{37} \]

where the latter equality follow from \(|H>| being a singlet, yielding \(< (m_z)^2 > = \frac{1}{3}m^2.\)

The above inequality (37) is an upper bound for \( Z_Q \), but represents an exact equality in the infinite size limit. In fact after a little algebra the state (28) with \(|i>| = |H>| saturates the bound (37), and represents the true eigenstate with momentum \( Q \) within the only assumption that the finite size gap in each sector of definite total spin and momentum scales as \( \frac{1}{l} \) (see App.VIII B). This basic assumption has been verified numerically as it is shown in Fig. 1 for \( t = 0 \) and \( \frac{J}{t} = 2 \) for various momenta. In particular in the static limit \( t = 0 \) the spin wave prediction of this gap always underestimates the value of the true gap computed by exact diagonalization on small lattices. In spin wave theory this gap scales as \( \frac{1}{l} \) since the perturbation induced by the hole affects only by small shift the bare spin wave energy excitation \( \epsilon_k \). The dispersion \( \epsilon_k \) depends linearly with momentum \( \epsilon_k \sim c|k| \), where \( c \) is the spin-wave velocity, and the lowest gap is given by \( \epsilon_k = \frac{2\pi}{l} \sim \frac{2\pi c}{l}. \) A plot of the quasiparticle weight for momentum \( Q = (\pi, \pi) \) is shown in Fig. 2 indicating that the finite size estimate of this quantity is strongly size dependent and without an exact result \( Z_Q = 2m^2 \) it would be difficult to decide whether \( Z_Q \) remains finite in the infinite size limit.

This is in general the case for \( J \neq 2t \), where the situation is still unclear and controversial so far.

The exact determination of the quasiparticle weight, obtained for particular wavevectors and \( J = 2t \) has evidenced a more general property of the Greens function in an insulator with long range magnetic order. In fact hole momenta differing by the antiferromagnetic wavevector \( Q \) are in general characterized by the same energy in the infinite size limit, but with a quite different quasiparticle weight. The two one hole eigenstates with momenta \( p \) and
$p + Q$ inside or outside the magnetic Brillouin zone respectively, have in fact a substantially
different overlap with the Heisenberg ground state, because they are essentially derived from
two orthogonal states: the Heisenberg ground state, and the corresponding lowest triplet
excitation, respectively. This property is clearly a general one, valid for all momenta: In
fact the relation between the lowest singlet eigenstates of $H^\text{eff}_p$ can be written, analogously
to Eq. (28),:

$$|S >_{p+Q} = \frac{2}{m} (\vec{S}_O \cdot \vec{m}) |S >_p$$

At the boundary of the magnetic Brillouin zone, momenta differing by $Q$ are equivalent by
spatial symmetries. Then arbitrary close to this surface there should be at least a singularity
in the quasiparticle weight, because the lowest energy state change dramatically even with an
arbitrary small variation of momentum. It is reasonable to expect a jump of the quasiparticle
weight that according to (37) is given approximately by:

$$\frac{Z(p + Q)}{Z(p)} \sim (2m)^2 = 0.37$$

where we have used that in the Heisenberg antiferromagnet the numerical value for the 2D
order parameter is $m \simeq 0.305$. [21]

**VII. CONCLUSIONS**

In this work I have discussed a general property of quantum antiferromagnets that can be
detected by well resolved photoemission experiments that are determined by the low energy
dynamic of a single hole in the undoped material.

Contrary to the existing folklore considering the single hole problem as an old, boring
and solved issue [5,9], it is found here that at least an effect has been overlooked by the
previous literature, effect that has been recently observed in the photoemission experiments
by Wells et al. and were independently predicted in [21].

Such experiments have evidenced the surprising effect that the photoemission spectra of
a quantum antiferromagnet apparently show up the presence of a Fermi surface as in the
corresponding metal at finite doping.

In the present work this fact is a consequence of a zero-energy magnon excitation carrying the antiferromagnetic-wavevector momentum and having an infinite lifetime in an antiferromagnet. This magnon is present in the ground state of the hole for momenta outside the Brillouin zone, while is absent in the other momentum region. The matrix elements entering in the spectral weight measured experimentally is jumping discontinuously along the mentioned surface separating the two momentum regions. This effect is just indicating the presence of this anomalous excitation.

This kind of excitation is washed out in any mean field treatment since as discussed in the introduction, in such a case the direction of the order parameter is fixed and the spin is no more a measurable quantity.

ACKNOWLEDGMENTS

I acknowledge useful correspondence of unpublished work by A. Parola who pointed out first the effective spin hamiltonian \(20\) in 1991. I am also grateful to E. Tosatti, M. Rice, A. Angelucci, D. Poilblanc, P. Prelovcek, P. Horsch and M. Muramatsu for useful discussions or comments.

VIII. SOME EXACT RESULTS FOR \(S = \frac{1}{2}\)

Consider the effective hamiltonian \(20\) for the single hole problem:

\[
H_p = H^t_p + H^J
\]

\[
H^t_p = t \sum_{\tau_\mu} e^{i p_{\tau_\mu}} \chi_{O,\tau_\mu} T_{\tau_\mu}
\]

\[
H^J = \frac{J}{2} \sum_{\langle R_i, R_j \rangle \neq O} (\chi_{R_i, R_j} - \frac{1}{2})
\]

\(H^J\) represents the translation invariant Heisenberg hamiltonian without all the bonds connecting the origin of coordinates \(O\). The single hole hamiltonian commutes with the total spin.
\[ S_{\text{tot}} = \sum_R \vec{S}_R \]  

(41)

and the spin at the origin \( \vec{S}_O \), whereas the operator \( \vec{S}_Q = \frac{1}{\sqrt{L}} \sum_R e^{-iQ R} \vec{S}_R \) defines long range order on a state \( |\psi> \) if \( <\psi| \vec{S}_Q \cdot \vec{S}_Q |\psi> \rightarrow m^2 L \) for \( L \rightarrow \infty \), where \( L \) is the number of sites, and \( m > 0 \) is the value of the order parameter.

We want to prove the following theorem:

**Theorem.** Given a single hole eigenstate \( |p> \) of the hamiltonian \( H_p \) with \( S_{\text{tot}} = 0 \), and energy \( E_p \), assuming that long range order exists in the given state for momenta \( Q = (\pi, \pi, \ldots) \), corresponding to antiferromagnetic long range order, then the triplet states:

\[ |\psi^j> = S^j_Q |p> \quad j = 1, 2, 3 \]  

(42)

define a state of the hamiltonian \( H_{p+Q} \) with energy expectation value

\[ E_j = \frac{<\psi^j|H_{p+Q}|\psi^j>}{<\psi^j|\psi^j>} = E_p + \frac{A}{L} \]  

(43)

where the constant \( A \) is given by:

\[ A = \frac{-4E_p + 2 \langle p| \sum \tau_\mu e^{ip\tau_\mu} |p>}{m^2 L} \rightarrow 4 \frac{e_p}{m^2} \]  

(44)

where \( -e_p < 0 \) is the ground state energy per site of the Heisenberg model obviously independent of \( p \). The latter limit is easily obtained, from the definition (44) since \( T_{\tau_\mu} \) has all eigenvalues bounded by one.

**Proof.** Since \( |p> \) is a singlet \( <\psi^j|\psi^j> = \frac{1}{3} Lm^2 \) is independent of \( j \), as well as \( E_j \). Then we consider the following operator:

\[ F = \sum_j F^j = \frac{1}{2} \sum_j \left[ S^j_Q (H_{p+Q} S^j_Q - S^j_Q H_p) + (S^j_Q H_{p+Q} - H_p S^j_Q) S^j_Q \right] \]  

(45)

By the exact relation:

\[ S^j_Q H_{p+Q} S^j_Q = \frac{1}{2} (H_p S^j_Q S^j_Q + S^j_Q S^j_Q H_p) + F^j \]  

(46)

, using that, by assumption, \( H_p |p> = E_p |p> \) it easily follows that:
\[ \frac{1}{3} \sum_j E_j = E_p + \frac{<p|F|p>}{<p|\vec{S}_Q \cdot \vec{S}_{-Q}|p>} \]  

(47)

Moreover from \( T_{\tau_\mu} S_Q = -S_Q T_{\tau_\mu} \) and:

\[ [S_Q^i, [\chi_{R_i,R_j}, S_Q^i]] = -\frac{8}{L} (S_{R_i} \cdot S_{R_j} - S_{R_i}^j S_{R_j}^i) \]  

(48)

yielding for \( S = 1/2 \):

\[ \sum_j [S_Q^i, [\chi_{R_i,R_j}, S_Q^i]] = -\frac{8}{L} (\chi_{R_i,R_j} - 1/2), \]

and the following expression for \( F \) holds:

\[ F = \frac{t}{2} \sum_j \sum_{\tau_\mu} e^{ip\tau_\mu} \left[ S_Q^i, [\chi_{O,\tau_\mu}, S_Q^i] \right] T_{\tau_\mu} + \frac{1}{2} \left[ S_Q^i, [H^J, S_Q^i] \right] = -\frac{4}{L} H_p + \frac{2t}{L} \sum_{\tau_\mu} e^{ip\tau_\mu} T_{\tau_\mu} \]

Finally using the above two relations and the fact that \( E_j \) is independent of \( j \) the statement is easily proven (43).

A. Consequences and remarks

Suppose that the state with momentum \( p \) is the lowest energy state within the restriction of momenta \( p \) and \( p + Q \) in the Brillouin zone, and suppose that this lowest energy \( E_p \) is obtained when the total spin is minimum \( S = 0 \), it will be shown that normalized singlet state defined in terms of \( \vec{m} = \frac{1}{\sqrt{L}} \vec{S}_Q \):

\[ |p + Q> = \alpha_L (\vec{S}_O \cdot \vec{m})|p> \]  

(49)

has an energy expectation value \( \bar{E}_{p+Q} = <p + Q|H_{p+Q}|p + Q> \) arbitrary close to \( E_p \) and yielding the following bounds for the lowest energy \( E_{p+Q} \) with momentum \( p + Q \) in the singlet subspace:

\[ E_p \leq E_{p+Q} \leq E_p + \frac{3A}{L} \]  

(50)

Proof. From:
\[(\vec{S}_O \cdot \vec{m})^2 = \frac{1}{4}m^2 + \frac{1}{L}(\vec{S}_O \cdot \vec{m}) - \frac{1}{2L^2}(\vec{S}_O \cdot \vec{S}_{tot}) \] (51)

the normalization constant is given by \(\alpha_L = \frac{2}{m} + O(\frac{1}{L})\) (the expectation value of \((\vec{S}_O \cdot \vec{m})\) on the singlet state \(|p\rangle\) can be bounded using the Schwartz inequality for fixed component \(j\): \(< p|(\vec{S}_O \cdot \vec{m})|p\rangle = 3 < p|S_{ij}^j m^j |p\rangle ≤ \frac{3}{2}m\) Consider now the normalized state:

\[|j\rangle = \sqrt{3\alpha_L}S_{ij}^j m^j |p\rangle \] (52)

This state has non vanishing overlap with the corresponding singlet one \(|p + Q\rangle\):

\[a_0^2 = |< j|p + Q \rangle|^2 ≥ (\text{Re} < j|p + Q \rangle)^2 = \frac{1}{3} + O(\frac{1}{L}).\]

Since the hamiltonian commutes with \(\vec{S}_O < j|H|j\rangle = \frac{< p | S_{ij}^j H S_{ij}^j |p\rangle}{< p | S_{ij}^j S_{ij}^j |p\rangle}\) which corresponds exactly to \(E_j\) in the previous theorem. By applying the theorem

\[< j|H|j \rangle = E_p + A/L \]

On the other hand the state \(|j\rangle\) can be written as \(|j\rangle = a_0|p + Q \rangle + |\psi'\rangle\) where the state \(\psi'\) has no component in the singlet and \(< \psi'||\psi'\rangle = 1 - a_0^2\). By hypothesis this state has an energy expectation value \(\frac{< \psi'||H||\psi'\rangle}{< \psi'||\psi'\rangle}\) higher than \(E_p\), the minimum possible energy between the \(p\) and \(p + Q\) subspaces. Thus using the conservation of the spin, it follows that:

\[E_p + A/L = < \mu|H|\mu > ≥ a_0^2 \tilde{E}_{p+Q} + (1 - a_0^2)E_p\]

where \(\tilde{E}_{p+Q} = < p + Q|H|p + Q \rangle\) is a variational estimate of \(E_{p+Q}\). Finally it the latter inequality gives:

\[E_p ≤ E_{p+Q} ≤ \tilde{E}_{p+Q} ≤ E_p + 3A/L \]

which concludes this proof.

Remark. The theorem is more generally valid even when the lowest energy state is no more a singlet state provided the energy gain to the \(S = 1\) and \(S = 2\) vanishes at least as \(\frac{1}{L}\). In fact the trial states \(|j\rangle\) have component only in the \(S = 0\), \(S = 1\) and \(S = 2\) sectors.
B. Exact variational state

It has been shown in the previous section that the variational state $|p + Q>$, defined in the singlet subspace is arbitrarily close in energy to the exact lowest energy singlet state $|\psi_{p+Q}>$ with momentum $p + Q$. It is reasonable to assume that the finite size gap in each subspace with definite spin and momentum is of the order $\sim 1/l$ because it is determined by an excitation of at least one magnon (remind that the spin wave excitations are of order $c|k|$, where $c$ is the spin wave velocity and the minimum allowed $|k| > 0$ is of order $1/l$). If the above hypothesis is correct as it can be easily verified numerically (see Fig. 1) it is possible to show rigorously that the variational state $|p + Q>$ is arbitrarily close to the exact eigenstate $\psi_{p+Q}$.

In fact suppose $|p + Q> = a_0|\psi_{p+Q}> + |\psi'>$, where by definition $|\psi'>$ is orthogonal to the lowest state with definite spin and momentum, and thus satisfying by assumption:

$$<\psi'|\psi'> = 1 - a_0^2$$
$$\frac{<\psi'|H|\psi'>}{<\psi'|\psi'>} \geq E_{p+Q} + B/l$$

Then it easily follows that:

$$<p + Q|H|p + Q> = a_0^2E_{p+Q} + (1 - a_0^2)(E_{p+Q} + B/l) = E_{p+Q} + (1 - a_0^2)B/l.$$  

The previous relation is compatible with the previously stated theorem only if

$$1 - a_0^2 = <\psi'|\psi'> \leq \frac{3Al}{BL} \to 0$$

which proves the statement of this section for $d > 1$, as $L = l^d$. 

25
REFERENCES

[1] B.O. Wells et al. Phys. Rev. Lett. 74, 964 (1995); Z.-X. Shen, W. E. Spicer, D. M. King, D. S. Dessau, and B. O. Wells, Science 267, 343 (1995).

[2] P. Aebi et al. Phys. Rev. Lett. 72, 2757 (1994).

[3] S. Chakravarty et al. Phys. Rev. Lett. 60, 1057 (1998).

[4] A. Parola and S. Sorella, Phys. Rev. B 45, 13156 (1992); S. Sorella and A. Parola, J. Phys. Cond. Mat. 4 3589 (1992).

[5] C.L. Kane, P.A. Lee and N. Read, Phys. Rev. B 39, 6880 (1989), S. Schmitt-Rink, C. M. Varma, and A. E. Ruckenstein, Phys. Rev. Lett. 60, 2793 (1988).

[6] G. Martinez and P. Horsch, Phys. Rev. B 44, 317 (1991).

[7] Z. Lin and E. Manusakis Phys. Rev. B 44, 2414 (1991).

[8] A. Angelucci, S. Sorella and D. Poilblanc, Phys. Lett. A 198, 145 (1995).

[9] B.I. Shraiman, E.D. Siggia Phys. Rev. B 42, 2485 (1990).

[10] see e.g. F. Strocchi “Elements of Quantum mechanics of infinite systems” World Scientific, Singapore (1985).

[11] H. Neuberger, T. Ziman, Phys. Rev. B 39, 2608 (1989).

[12] B. Bernu, C. Lhuillier, and L. Pierre Phys. Rev. Lett. 69, 2590 (1992).

[13] P. A. Bares, G. Blatter and M. Ogata Phys. Rev. B 44, 130 (1991).

[14] E. Lieb and D. Mattis J. of Math. Phys. 3, 749, (1962).

[15] L. Faddeev, L. Takhtajan, Phys. Lett. A 85, 375 (1981).

[16] P.W. Anderson, Science 235, 1196 (1987).

[17] Q. F. Zhong and S. Sorella Phys. Rev. B 51 16135 (1995).
[18] D. J. Scalapino S. R. White and S. Zhang Phys. Rev. B 47, 7995 (1993).

[19] F.C. Zhang and T.M. Rice, Phys. Rev. B 37, 3759 (1988).

[20] Q.F. Zhong, S. Sorella, Europys. Lett. 21, 629 (1993).

[21] S. Sorella, J. Low Temperature Phys. 99, 371, (1995).
FIGURES

FIG. 1. Plot of the finite size gap to the first singlet excitation as a function of the inverse lattice side length in 2D for (a) the static limit $t = 0$, full dots are obtained by numerical diagonalizations and triangles represent the spin-wave predictions, (b) $J = 2t$ and momentum $p = (0,0)$. In this case also the gap to the lowest $S = 3/2$ excitation of the Heisenberg model scaling to zero as $\frac{1}{L}$ is shown for comparison (squares), while the triangles represent the corresponding gap for the Heisenberg lattice (without the hole) in spin-wave approximation. (c) $J = 2t$ and momentum $p = (\pi/2, \pi/2)$ corresponding to the single hole ground state. The triangles are the same points as in (b). (d) $J = 2t$ and momentum $(\pi, \pi)$. The triangles are the same points as in (b).

FIG. 2. Plot of the quasiparticle weight for momentum $p = (\pi, \pi)$ as a function of the lattice size for different values of $\frac{J}{t}$. The star indicate the expected asymptotic $L \to \infty$ value (see text) for $J = 2t$. 
Figure 1: Graph showing the relationship between $\Delta/t$ and $1/l$ for different values of $t/J$.

- **Lanczos** (solid circles)
- **Spin-Wave** (triangles)

The graph demonstrates a linear relationship with a single line for $t/J=0$.
$p = (\pi/2, \pi/2)$

(c)

S. Sorella  Fig. 1
