Hole Dynamics in a Quantum Antiferromagnet beyond the Retraceable Path Approximation

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**Abstract**

The one-hole spectral weight for two chains and two dimensional lattices is studied numerically using a new method of analysis of the spectral function within the Lanczos iteration scheme: the Lanczos spectra decoding method. This technique is applied to the $t-J_z$ model for $J_z \to 0$, directly in the infinite size lattice. By a careful investigation of the first 13 Lanczos steps and the first 26 ones for the two dimensional and the two chain cases respectively, we get several new features of the one-hole spectral weight. A sharp incoherent peak with a clear momentum dispersion is identified, together with a second broad peak at higher energy. The spectral weight is finite up to the Nagaoka energy where it vanishes in a non-analytic way. Thus the lowest energy of one hole in a quantum antiferromagnet is degenerate with the Nagaoka energy in the thermodynamic limit.

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After the discovery of superconductivity in materials which exhibit antiferromagnetic (AF) long range order in the insulating phase, much attention has been given to the study of strongly correlated system at low doping. Despite the enormous amount of work, the dynamical properties of one hole in a quantum antiferromagnet (QAF) are still a subject of debate [1–3].

A satisfactory model of a QAF is provided by the Heisenberg hamiltonian which, in 2D, is known to show Néel long range order. In the following we mimic the properties of a QAF by use of the simpler AF Ising hamiltonian whose exact ground state is the Néel state and we address the problem of the propagation of a hole in the $J_z \rightarrow 0$ limit of the $t-J_z$ model defined by:

\[ H = -t \sum_{<i,j>,\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) + J_z \sum_{<i,j>} S_i^z S_j^z \quad (1) \]

where the constraint of no double occupancy is understood. Both the two chain (2C) and the two dimensional square lattice (2D) will be considered. The Nagaoka (NK) theorem [4], provides a lower bound $e_F$ to the ground state energy of one hole in the $J_z \rightarrow 0$ limit:

\[ e_F = -zt, \]

where $z$ is the coordination number of the lattice ($z = 3$ for the 2C problem and $z = 4$ for the 2D case).

A complete description of the one particle spectrum, not limited only to the ground state, was first given in the seminal work of Brinkman and Rice (BR), where the so called “retraceable path approximation” (RP) was introduced [5]. In this approximation the spectral weight is completely incoherent and the hole is essentially localized without dispersion. The RP is exact in 1D (where NK theorem does not apply) and recently it has also been shown to be exact in the limit of infinite spatial dimensionality [6,7]. However, no analytical solution is available for finite $z > 2$ and it is not clear how accurate the RP is in these cases. Indeed, in finite dimensions $D > 1$ several one hole paths exist, allowing for the propagation of the hole [8].

Recently, the problem of hole propagation has been addressed by use of the quite efficient Lanczos technique in 2D lattices with up to 26 sites [2] or with a promising approximate
technique up to 50 sites \[\text{[8]}\]. Despite the remarkable numerical effort, still the number of sites appears to be too small for a precise determination of the properties of the spectral function or for the ground state properties for \(J_z \to 0\).

In this work, we present a numerical study of the one hole spectral weight by means of the Lanczos iteration scheme, applied directly to the infinite system \[\text{[9]}\]. We introduce a new method for the calculation of the spectral weight, that we name the Lanczos spectra decoding method (LSD). This new method combines the power of the Lanczos algorithm with some general properties of the spectral function.

As well known, the Lanczos technique consists of a partial diagonalization of the hamiltonian in the basis generated by the vectors \(s_n = H^n |\Psi_T\rangle\) for \(n = 0, 1, ..., N\), where \(|\Psi_T\rangle\) is a trial state. After orthogonalization of the vectors \(s_n\), the hamiltonian reduces to tridiagonal form and the resulting orthogonal basis \(\{e_i\}\) can be iteratively calculated \[\text{[10]}\]. In this restricted basis it is straightforward to compute static and dynamical correlation functions. Usually, convergence is reached for \(N\) much smaller than the dimension of the Hilbert space, justifying the success of the method. In an infinite system this procedure can be applied as well, provided the Hilbert space generated by the iterative application of \(H\) to the trial state remains finite. This is in fact the case for the “simple” \(t - J_z\) model if we consider the basis of states where the hole is located at the origin and the \(z\)-component of the spin is defined in any other site. The application of the hamiltonian to one of these states generates at most \(z\) new elements of the basis and, after \(N\) steps, the Hilbert space is finite having at most dimension \(z^N\). However, this exponential growth makes the problem intractable even for relatively small \(N\). Fortunately many of the generated states appear several times during the expansion process of the Hilbert space which in fact turns out to be considerably smaller than the previous estimate. Another reduction factor can be gained by implementing the translation symmetry of the hamiltonian. Translation operators can be always used to move the hole at the origin of the lattice and only the corresponding basis elements must be stored.

By applying the above strategy, the dimension of the Hilbert space grows much slower
than $z^N$ and in fact we are able to go up to $N = 26$ for the 2C case and $N = 13$ for the 2D case with an Hilbert space dimension at most equal to $\sim 12.2 \times 10^6$. The 2C model is much easier to study with this method, though the properties of the spectral weight are rather similar to the 2D case as we will show in the following. Further details of this calculation will be published elsewhere [11].

We apply the Lanczos algorithm to the $t - J_z$ model, using as trial state $|\psi_T\rangle$ the exact ground state of the undoped system with a hole of definite momentum $k$, i.e. $|\Psi_T\rangle = \frac{1}{\sqrt{L/2}} \sum_{R \in A} e^{i k \cdot R} c_{R\uparrow} |\Phi\rangle$ where $|\Phi\rangle$ is the Néel state with spin up electrons in the $A$ sublattice and $L$ is the size of the lattice, where periodic boundary conditions are assumed.

The spectral weight can be formally calculated at fixed $N$ and reads:

$$A(k, \omega) = \text{Im} \frac{1}{\pi} \left( \frac{1}{\omega - H - i\delta} \right) = \sum_{i=0}^{N} |\langle \Psi_i | \Psi_T \rangle|^2 \delta(\omega - E_i)$$ (2)

where $E_i$ and $|\Psi_i\rangle$ are eigenvalues and eigenstates of $H$ in the restricted Lanczos basis. We expect that for $J_z \to 0$ the spectral function is completely incoherent in the infinite size limit and we know that by the NK theorem $A(k, \omega)$ is identically zero outside the interval $e_F < \omega < -e_F$. As a result of the finiteness of our Hilbert space, at fixed $N$ we get a sum of $\delta$-functions in the spectral weight. This feature also appears in the exact spectral function of finite systems and, in that framework, an estimate of the thermodynamic limit is obtained by smoothing the $\delta$-functions in Eq. (2) with lorentzians of a given small width $\delta$: $\delta(\omega - E_i) \rightarrow \text{Im} \frac{\pi^{-1}}{\omega - E_i - i\delta}$. For small $\delta$ reasonable results can be obtained, provided the resolution of the energy levels becomes much smaller than $\delta$ for large $N$. In our case, however, we cannot reach very large $N$ and a more efficient method for evaluating the spectral weight is necessary. The $N \to \infty$ limit of the spectral function may contain a coherent part only if in this limit some $Z_i = |\langle \Psi_i | \Psi_T \rangle|^2$ attains a finite value. We have verified that for both the 2C and the square lattice, all $Z_i$ tend to zero and therefore the spectral function is completely incoherent as expected. The spectral weight can be always written as a product of two functions:
\[ A(k, \omega) = Z(\omega) \rho_L(\omega) \]  

where

\[ \rho_L(\omega) = \frac{1}{N+1} \sum_{i=0}^{N} \delta(\omega - E_i) \]  

and \( Z(\omega) \) is defined at discrete points:

\[ Z(\omega) = (N + 1)|\langle \Psi_i | \Psi_T \rangle|^2 \]  

for \( \omega = E_i \). If \( A(k, \omega) \) is incoherent and the Lanczos eigenvalues are set in ascending order \( E_{i+1} > E_i \), \( Z(\omega) \) describes a well behaved function of \( \omega \) as well as the coarse grained Lanczos density of states (LDOS) which can be estimated from Eq. (4) as

\[ \rho_L(\bar{\epsilon}_i) = \frac{E_i + E_{i+1}}{2} = \frac{1}{(N + 1)(E_{i+1} - E_i)}. \]  

Analogously, \( Z(\omega) \) can be then interpolated linearly at energies \( \bar{\epsilon}_i \):

\[ Z(\bar{\epsilon}_i) = (Z_{i+1} + Z_i)/2. \]  

Eqs. (3,4) are accurate to \( O(1/N^2) \) and better fits are possible using more data for the interpolation procedure. \( A(k, \omega) \) easily follows from Eq. (3). At the end, we can verify the sum rule \( \int A(k, \omega) d\omega = 1 \), as a check for the accuracy of the calculation. This is all about the LSD method.

In order to test LSD we have applied it to an exactly solvable problem. If we neglect all closed paths in the averages of \( < \psi_T | H^n | \psi_T > \) the resulting Green’s function is the known BR one. On the other hand, this is the exact Green’s function in the Bethe lattice of coordination \( z \). LSD is perfectly defined in this case. In fact, it is possible to compute analytically \( Z \) and \( \rho_L \) in Eqs. (3,4) due to the simple structure of the Lanczos matrix in the Bethe lattice case: \( \langle e_i | H | e_{i+1} \rangle = \sqrt{z-1} \) for \( i > 0 \) and \( \langle e_0 | H | e_1 \rangle = \sqrt{z} \) are the only non-zero upper diagonal matrix elements in the orthogonal Lanczos basis \( \{ e_i \} \).

In Fig. 1 we show a comparison of the spectral weight obtained by smearing out the \( \delta \)-functions–usual method– and by applying our scheme. We see that the agreement of
our data with the exact results is very good and we easily resolve the first peak in $A(\omega)$ (dispersionless in this case) for the 2C case. By contrast the usual method cannot give accurate results with the available number $N$ of Lanczos steps.

In the following, we present the results for the 2C and the 2D case, obtained using this new method to evaluate the spectral weight, without any approximation. We show in Fig. 2 the spectral weight for $k = (0, 0)$ obtained with different numbers of Lanczos steps. For the 2C case, our results are well converged and we find a sharp peak located at an energy close to the BR one $e_{BR} = -2t\sqrt{z-1}$ and, surprisingly, a second peak at energy $\sim -t$. In the 2D case, the spectral weight looks similar, although the first peak is rather small.

In 1D, the exact BR solution leads only to one peak but with a divergent spectral weight $\sim \frac{1}{\sqrt{\omega_c - \omega}}$ at the bottom $\omega_c$ of the band. Already in the 2C case such a divergence disappears within the RP, as well as in our numerical scheme, which includes all closed-loop paths. In fact the peak in Fig. 2 does not depend much on the number $N$ of Lanczos steps.

In Fig. 3 we see that the first peak in the spectral function has a remarkable dispersive feature although the bottom of the spectrum appears $k$–independent. The dispersion of the first peak is not present neither in 1D or in infinite dimension [6,7] and the importance to go beyond the RP is clear even in 2D.

The one particle density of states (DOS) can be computed either by integrating $A(k, \omega)$ over $k$ or equivalently by a direct evaluation of $\text{Im}G(R = 0, \omega)$. As it is shown in Fig. 2 for the 2C case, our results present some small deviation to the DOS in RP approximation especially when large closed paths are allowed. In 2D however the BR solution seems already quite accurate, at least away from the band tails.

Another open problem is whether the band edge of a hole in a QAF coincides with the NK energy and how the spectral weight vanishes at the band edges. At finite $N$ the lowest eigenvalue of the hamiltonian $E_N$ restricted to the Lanczos basis is of course a variational upper bound to the lowest eigenstate non-orthogonal to $|\psi_T \rangle$. Note that the NK state is orthogonal to $|\psi_T \rangle$ only in the infinite system and $E_\infty = \lim_{N \to \infty} E_N$ may be different from $e_F$, contrary to the finite size case. Thus $E_\infty$ is a definition of the one hole energy in a
quantum antiferromagnet and since it coincides with the smallest energy $\omega$ where $A(k, \omega)$ vanishes. In order to have a good estimate of this energy $E_\infty$ it is useful to know what are the leading corrections of the quantity $\Delta_N = E_N - E_\infty$ for $N \to \infty$. The way $\Delta_N$ vanishes for $N \to \infty$ is related to the form of the LDOS at low energy. In the BR case the exact solution gives $\rho_L(\epsilon) \sim \epsilon^{-1/2}$ (see Fig.2). Thus, using Eqs. (6), $\Delta_N^{-1/2} \sim \frac{1}{\sqrt{N}}$, yielding $\Delta_N \sim \frac{1}{N^{1/2}}$. In the general case we have numerical evidence of a finite LDOS, and the same argument determines $\Delta_N \sim \frac{1}{N}$.

We have plotted in Fig.4(a) the estimated ground state energies as a function of $1/N$ for several momenta for the 2C case. Many of the estimated Lanczos energies – exact upper bound of the true ground state energy– are clearly below the BR energy (even for the 2D case not shown in the figure [11]). Thus, a previous suggestion that the one hole energy in a QAF should be close to $e_{BR}$ [12,[13] is not confirmed by our numerical results. In Fig.4(a) it is a remarkable property that all the extrapolated energies are very close to the NK energy, independent of the momentum of the hole, $E_\infty = -3 \pm 0.02$ although the spin configuration is antiferromagnetic. This clearly suggests that the spectral weight is finite up to the NK energy. Moreover the fact that the corresponding quasiparticle weight becomes very small close to the NK energy (e.g. $Z = 0.02$ for $E_{26} = -2.92$ and $p = 0$) may indicate that the vanishing of the spectral weight is non-analytic. Indeed a least square fit of our data for the band tail is more consistent with an exponential vanishing rather than with a power law.

In order to check the estimated $J_z \to 0$ energy we have also computed $E_N$ for the finite $J_z$ model, where due to the localization of the hole in the linear “string” potential $E_N$ converges exponentially with $N$ and $N = 26$ gives already a very accurate estimate (within 0.1 %) for $J_z > 0.1$. For smaller $J_z$ ( 0.02 $\leq$ $J_z < 0.1$ ) the same accuracy is obtained by fitting the Lanczos data with $\Delta_N \propto e^{-const. \frac{N}{J_z}}$, which interpolates consistently the $\Delta_N \to 0$ convergence in the limit $J_z = 0$ and in the finite $J_z$ case. In the string picture the one hole energy for small $J_z$ should be $E = a + b \frac{J_z^\theta}{t}$ with $a = e_{BR}$ and $\theta = 2/3$ independent of $z$. Our data shown in Fig. 4(b) are clearly consistent with the BR exponent 2/3, although $a = e_F$. The next leading corrections to the contribution $J_z^{2/3}$, are also very important. For small
$J_z$ in the 2C case we do not find any transition to a phase separated (PS) polaron state \cite{13}: $E_{PS} = -3t + c(J_z^2/3)$, with $c/t = 3(\pi/2)^2/3 = 4.05$. Previous numerical work \cite{14} is in qualitative agreement with our results although the small size studied \cite{14} was not enough to detect the $J_z \to 0$ smooth crossover to the NK energy, that we found in the 2C case.

In summary, we have presented here a successful attempt to go beyond the RP for the hole dynamics in a QAF. A new Lanczos-type of analysis of the spectral weight enabled us to get very accurate results for the 2C problem and qualitatively similar ones for the 2D case. A clear dispersion of the main incoherent peak of $A(k,\omega)$ both for the 2C and the 2D case was found. The variational argument about phase separation on the $t - J_z$ model (or $t - J$) for small $J_z$ was based on the assumption that the one hole energy in a QAF is smaller than the NK energy $e_F$ by a finite amount \cite{13}. Instead our results strongly suggest that $E_{\infty} = e_F$ for $J_z \to 0$. In fact as it is shown in Fig. 4(b) the one hole energy in a phase separated polaron is always well above the exact estimated ground state energy for all $J_z > 0.02$. Of course numerically we cannot rule out that a phase transition to a non-uniform phase may actually occur for unphysically small $J_z$. Anyway the fit of the energy data for small $J_z$ extrapolate to the $J_z = 0$ NK energy with a remarkable accuracy (see caption Fig. 4b).

Thus the phase separation in the small $J_t - J$ model may be washed out by quantum fluctuations \cite{15,16}, especially in higher dimensions where $E_{PS}$ approaches $e_F$ for $J_z \to 0$ with a much smaller exponent.

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FIGURES

FIG. 1. Comparison of the LSD for 10, 18 and 26 (8,11 and 13) Lanczos iterations with corresponding analytical results (solid lines) within the RP for the Bethe lattice with coordination number $z = 3$ ($z = 4$). Triangles, squares and circles correspond to the small, medium and large $N$ calculation respectively. The long dashed lines and dashed-dot lines are fit of $A(\omega)$ obtained by the standard method (see text) with $\delta = 0.05$ and $\delta = 0.1$ respectively.

FIG. 2. Calculated $k = 0$ -spectral weight and DOS for $N = 10, 18, 26$ (8,11,13) for the 2C (2D) model. Solid lines are cubic interpolations of the largest $N$, and the dashed lines are the BR densities of states and a guide to the eye for the 2D-$A(k, \omega)$. The symbols for the points are as in Fig.1.

FIG. 3. Calculated momentum dependent spectral function (lower part) for different $k$ in the magnetic Brillouin zone and the dispersion of the first peak for the same $k$ values (upper part). The bars are typical estimates of the first-peak width. For the 2C $A(k, \omega)$, the wavevector $k$ ranges from from $(0,0)$ (bottom) to $(\pi,0)$ (top) with nine equally spaced values. For each $k$, we have shifted the spectral function by 0.25 successively. For the 2D $A(k, \omega)$ the $k$−path in the magnetic Brillouin zone is shown in the inset The inset in the 2C dispersion is the free electron behavior.

FIG. 4. (a):Plot of the lowest eigenvalues of the 2C model as a function of $1/N$, the inverse of the Lanczos iteration number, for the same momenta shown in Fig.3. The horizontal dashed lines is the BR ground state energy. (b): ground state energies (crosses) vs $J_z^{2/3}$ for the 2C model. The continuous line connects linearly the data and the dotted line is an extrapolation ( consistent with the RP [7]) of the last five points for $J_z \to 0$: $E(J_z) = E(0) + a \frac{J_z^{2/3}}{t} + b J_z$, with $a/t = 2.6$, $b = -2.2$ and $E(0) = -2.996t$. The long dashed line is the polaron energy (see text).