Single hole in a quantum antiferromagnet: Finite-size-scaling approach

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Exact diagonalizations of small clusters up to 26 sites are used to extrapolate the ground-state energy of a single hole in the Néel state of the t-J_z model or in the quantum antiferromagnetic (t-J model). A surprisingly rapid convergence with system size is observed for a wide range of parameters and for the largest clusters considered. In the Ising limit the energy dependence with J_z is remarkably close to a $J_z^{2/3}$ law for intermediate coupling in agreement with Brinkman-Rice type of calculations. Nevertheless a small but significant bandwidth indicates that the hole can propagate coherently in this limit. Clearly the polaronic behavior $\sim J_z^{1/2}$, for very small J_z, is out of the range of the method. When quantum fluctuations are introduced (isotropic case) the ground-state energy behavior still remains close to that of the Ising limit although an overall increase of the energy by a factor $0.3t$ is observed. This suggests that the "string scenario" might have some relevance there.

The recent discovery of the high-T_c superconducting copper oxydes has motivated a huge theoretical effort in the field of strongly correlated fermions on two-dimensional lattices. Apart from the well-known Nagaoka theorem[1] almost no exact results exist for this problem in two dimensions (2D). Furthermore, validity of perturbation expansions still remains controversial. Therefore, in the last five years a large effort in developing numerical methods has been made. Based on the Lanczos algorithm, exact diagonalization (ED) techniques have proven to be very successful in investigating both static and dynamical properties of strongly correlated Hamiltonians in one or two dimensions. Contrary to quantum Monte Carlo (QMC) methods ED do not show any sign of instability. However, ED has been restricted so far to quite small systems, typically 4×4 clusters, owing to the exponentially fast growth of the Hilbert space with the system size. Furthermore, no real finite-size scaling approach has ever been undertaken apart from the undoped case.[2] The aim of this paper is to initiate such a finite-size scaling analysis in the case of a single hole moving in an antiferromagnetic background.

Although the single-hole problem is one of the simplest problems that one can think of, it is nevertheless a very tough one (in 2D) for which there are very few firm results. The relevant Hamiltonian in the strong-coupling limit is defined as follows:

$$\mathcal{H}=J_z\sum_{\mathrm{i},\vec{\epsilon}} S_{\mathrm{i}}^z S_{\mathrm{i}+\vec{\epsilon}}^z+\tfrac{1}{2}J_\perp\sum_{\mathrm{i},\vec{\epsilon}}(S_{\mathrm{i}}^+S_{\mathrm{i}+\vec{\epsilon}}^-+S_{\mathrm{i}}^-S_{\mathrm{i}+\vec{\epsilon}}^+) -t\sum_{\mathrm{i},\vec{\epsilon},\sigma}(\tilde{c}_{\mathrm{i},\sigma}^\dagger\tilde{c}_{\mathrm{i}+\vec{\epsilon},\sigma}+\mathrm{H.C.})\ , \qquad (1)$$

where $\vec{\epsilon}=\vec{x}$ and $\vec{y}$ and $\tilde{c}_{\mathrm{i},\sigma}^\dagger=(1-n_{\mathrm{i},-\sigma})c_{\mathrm{i},\sigma}^\dagger$ is the projected fermion operator which enforces the constraint of the electron density $n_{\mathrm{i},\sigma}$ at all sites i to be either 0 or 1 (doubly occupied site are projected out). The rest of the notation is standard. The antiferromagnetic coupling J between nearest-neighbor spins has been separated into its diagonal and transverse components J_z and $J_\perp$, respectively. $J_\perp=0$ corresponds to the Ising limit and $J_\perp=J_z=J$ to the isotropic case; we shall study both cases in the following. Hereafter we set $t=1$.

Even when quantum spin fluctuations are included ($J_\perp=J_z$), we expect long-range antiferromagnetic order in the zero hole concentration limit (corresponding to a single hole in an asymptotically large system). The complexity of our problem is closely related to the inherent coupling between the spin and the charge degrees of freedom, in the sense that the moving hole perturbs the underlying antiferromagnetic background. In the Ising limit $J_\perp=0$, and for J_z not too small ($10^{-2}<J_z<1$) one can assume that the Néel arrangement of the spins is basically preserved even in the vicinity of the moving hole. The excursion of the hole away from the origin would then lead to a string of overturned spins. Clearly to remove the string, in the simplest approximation, the hole has to retrace its path.[3] For nonzero J_z the magnetic energy grows linearly with the length of the string.[4,5] The hole is then localized at the origin by a linear potential. This results in a series of localized levels[4,5] and a hole GS energy behaving as[4]

$$\epsilon_h=E_0-E_{\mathrm{Ising}}\sim -2\sqrt{3}+2.74J_z^{2/3}\ . \qquad (2)$$

Above and throughout the paper the hole GS energy is measured from the energy reference of the undoped case, E_{Ising} or E_{Heis}, for $J_\perp=0$ and $J_\perp=J_z$, respectively. Early ED and QMC studies[6] confirm the behavior (2). Although the string picture strictly predicts a localized hole wave function, some high-order processes allow a coherent motion of the hole in a narrow band.[7,8] Indeed the process that consists of six successive hops of the hole around the plaquette does not lead to any frustration in the spin background in the final state, and gives rise to an effective hopping along the diagonal of the plaquette. For very small J_z a polaronic regime[4,6] is expected with a distortion of the spin background on a large disk of radius growing as $J_z^{-1/2}$ and a hole energy

$$\epsilon_h\sim -4+6.03J_z^{1/2}\ . \qquad (3)$$

This results from a simple equilibration between the delocalization energy of the hole and the magnetic-energy cost of the spin-disordered region. For $J_z=0$ the Nagaoka ferromagnet[1] of energy -4 is then recovered. In Fig. 1 we show the two results (2) and (3). One clearly sees that the polaron effect is only of importance for extremely small J_z ($J_z<0.02$), whereas otherwise the delocalization due to motion along strings (or self-retracing paths) contributes most of the energy.

The isotropic case $J_\perp=J_z$ is much more subtle since the spin fluctuations can repair the damage along the string of the hole flipping back the overturned spin. Therefore, the string scenario seems *a priori* to lose its relevance here since the hole no longer sees any potential barrier. However, earlier numerical calculations[9,8,10] reveal that the hole energy still exhibits a behavior close to $J^{2/3}$, which is compatible with the string picture provided that the correct spin-spin correlations of the Heisenberg Hamiltonian are taken into account.[11]

There is so far no estimate of the finite-size corrections that may well play a very important role for small cluster calculations. It is thus clearly interesting to extend previous work to larger clusters. As will be seen, one can then use the variation of physical properties with system size to obtain rather well-defined results. In the following, we show ED results of small 2D clusters of increasing size N but with a fixed hole number $N_h=1$. Our aim is to try to extrapolate various quantities to the thermodynamic limit $N\to\infty$ that would correspond to a vanishing hole density. If no simple scaling law exists we shall however be able to give good estimates for the extrapolated values (or in some cases rigorous upper or lower bounds). Periodic boundary conditions (BC) are used and we restrict ourselves to clusters of square geometry in order to obtain smooth behaviors with increasing system size. The cluster shape is determined by two orthognal translation vectors $\mathbf{T}_1=(n,m)$ and $\mathbf{T}_2=(-m,n)$, where n and m can be any integer, and the number of nonequivalent sites is then $N=n^2+m^2$. It is also required that N is even to avoid frustration of the antiferromagnetic spin background. In other words, the antiferromagnetic wave vector $\mathbf{Q}_0=(\pi,\pi)$ shall always belong to the (discrete) reciprocal space. According to these rules, cluster sizes that can be considered are $N=8$, 10, 16, 18, 20, 26, 32, ... Clearly

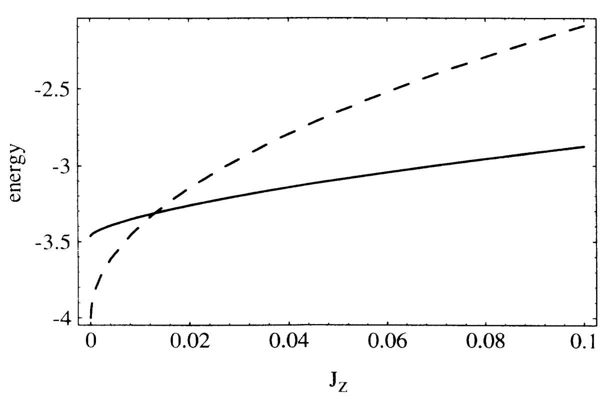

FIG. 1. Hole energy vs J_z in the polaron picture (dashed curve) and in the string picture (solid curve). Here and throughout the paper energies are measured in units of t.

$N=8$ is too small to be of interest and $N=32$ is too large to be handled by present-day computers. The Hamiltonian is diagonalized by a Lanczos procedure in the $S_z=\frac{1}{2}$ sector. In the isotropic case this can always be assumed because of spin rotational invariance. Translation symmetries are also used to further block diagonalize the Hamiltonian. Note that, since we are interested in the GS in every sector of the momentum $\mathbf{k}$ belonging to the reciprocal lattice, the C_4 group symmetries of the lattice (compatible with the cluster square shape) cannot in general be used.[12] For the larger cluster of $N=26$ sites the relevant Hilbert space is span by a basis of $\sim 5.2\times10^6$ configurations. In general the Lanczos vectors are complex vectors in the basis of configurations so that real tables of size 10^7 are necessary for the representation of each of them. The Hamiltonian matrix occupies around 2 Gbytes of disk space and the basic matrix vector multiplication takes around 2 min of CPU on a Cray-2 supercomputer.

Let us now first discuss the results obtained for $J_\perp=0$. Since the Ising term of the Hamiltonian breaks spin rotational invariance the total spin $\mathbf{S}^2$ is not a good quantum number (contrary to the z-component S_z). This means that the GS is a combination of all the various spin components. Numerical evidence indicates[6] that the GS belongs to the $S_z=\frac{1}{2}$ sector so that the diagonalization of (1) has been restricted to this subspace. We found that, whatever N or J_z, the GS has a total momentum $\mathbf{Q}=\mathbf{0}$ and is fully symmetric with respect to 90° rotations. It is quite remarkable that no level crossing occurs down to $J_z=0$. This can be seen in Fig. 2(a) from the smooth behavior of the GS energy with J_z. At $J_z=0$ the Nagaoka theorem[1] holds and the GS is the fully polarized ferromagnet in the $S_z=\frac{1}{2}$ sector. With increasing J_z the weights of the smaller spin components increase smoothly.[13] For small J_z the energy varies linearly $\sim -4+(N/2)J_z$ as speculated in Ref. 6. It means that for $N\to\infty$ the slope $\partial\epsilon_h/\partial J_z\to\infty$; this is a signature of the polaronic regime[4] with a $J_z^{1/2}$ behavior as mentioned above. Because of the prefactor of $N/2$ in the slope it is clear that no convergence of the energy can be obtained for, let us say, $J_z<0.1$ and $N\le 26$.

In the large-J_z limit, where a perturbation expansion in $1/J_z$ can be used,[6] $\epsilon_h\sim J_z-\frac{8}{3}J_z^{-1}+\alpha J_z^{-3}$. The first term comes from the energy lost in breaking four bonds and our numerical estimate for α is ~ 2.52.

Now let us concentrate on the intermediate J_z region ($J_z<1$). In Fig. 3 we can observe that the hole GS energy versus $1/N$ is very smooth and regular. This can also be seen in Fig. 2(a). Clearly if N is too small, finite-size corrections are of order N but for N larger than a critical size $N_c(J_z)$ the corrections seem to vanish more rapidly than any algebraic law $N^{-\gamma}$. Physically this happens when the cluster size becomes comparable to the extension of the hole wave function. Our data roughly suggest an estimate $N_c\sim 6J_z^{-2/3}$. Note that according to Ref. 4 the expected string length lies around $l\sim 1.9J_z^{-1/3}$, yielding a hole wave function of size $\pi l^2\sim 11J_z^{-2/3}$ compatible with $N_c(J_z)$. Consequently a very good convergence of ϵ_h is obtained at $N=26$ down to $J_z=0.25$. For $J_z\ge 1$ we

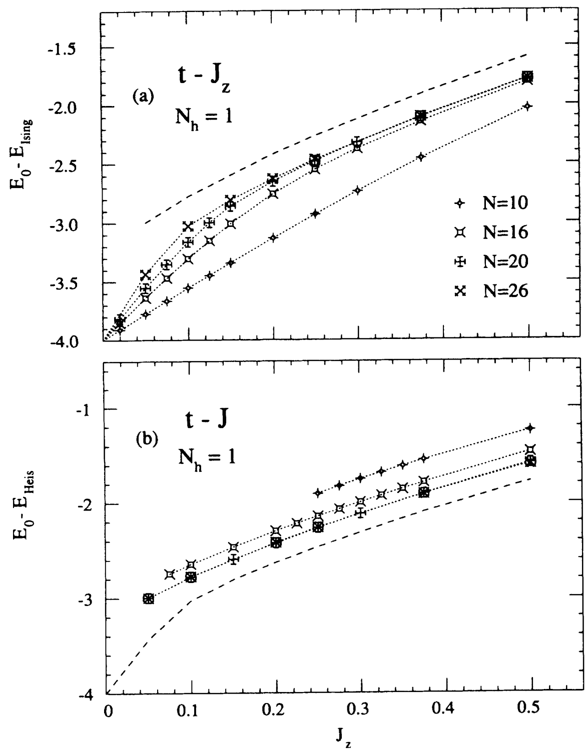

FIG. 2. Hole GS energy vs J_z for various cluster sizes; (a) Ising limit; (b) isotropic case. The dashed lines in (a) and (b) correspond to the data for $N=26$ for the isotropic and the Ising case, respectively. In (b) only the $S=\frac{1}{2}$ regime is considered above a small critical value of J.

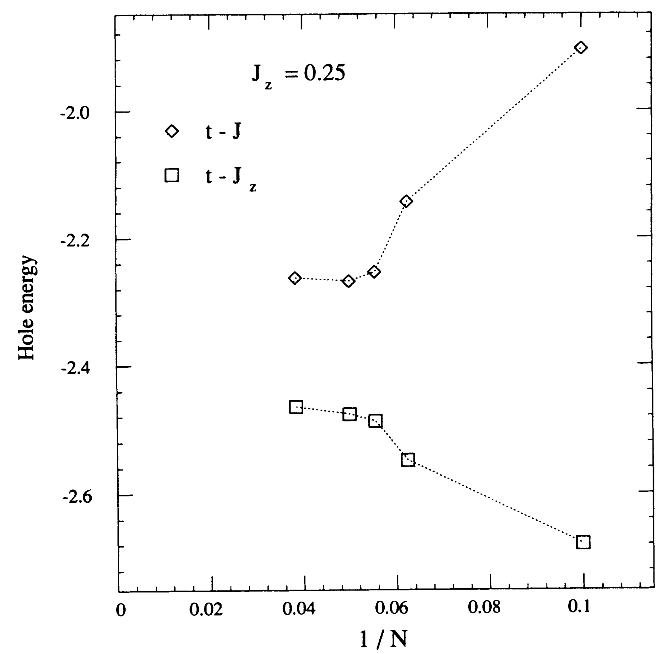

FIG. 3. Hole GS energy vs $1/N$ for $J_z=0.25$.

even obtain results accurate to more than 4 significant digits. This is shown in Table I where our Lanczos data for the two largest sizes are compared to the QMC data of Ref. 6. The agreement is good although statistical errors in the QMC data seem to be quite large [in particular, for $J_z=1$, comparing our results with the QMC data (Table I), it would seem that the QMC error bars are underestimated[14]].

Since ϵ_h has a square root behavior for small J_z and varies linearly at large J_z it is clear that a fit of the form

$$\epsilon_h \sim \beta + \delta J_z^{\nu} , \qquad (4)$$

where $0.5 < \nu < 1$, should apply in the intermediate-J_z regime. For $0.25 \le J_z \le 0.5$ a form like (4) is indeed excellent and yields

$$\nu \sim 0.653(2) , \quad \beta \sim -3.664(2) , \quad \delta \sim 2.967(6) , \qquad (5)$$

where the error is in the last digit. This is in good agreement with the fit based on QMC (Ref. 6) which predicted $e_h = -3.66 + 2.96 J^{0.655}$. The parameters (5) are also reasonably close to those of (2). This supports the suggestion that the hole creates a string of overturned spins leading to a confining potential. It should be clear from Fig. 1 that in this parameter region the polaronic effect is not expected to play any role. Finally let us mention that, already when J reaches 1, the fit (5) deviates from the exact GS energy as can be seen from a comparison with Table I.

Despite the rather accurate prediction for the GS energy the string picture (or retraceable path approximation) is unable to explain a possible coherent motion of the hole. Indeed, it implies instead that the hole is self-

TABLE I. Hole GS energy in the t-J_z model for several values of J_z. A comparison between our ED data with the QMC data of Ref. 6 is made. The ED data are lower bounds for the exact GS energy in the thermodynamic limit.

J_z	$N=20$	$N=26$	$N=6\times6$ (QMC)	$N=8\times8$ (QMC)
0.2	−2.649 054	−2.627 044	−2.631±0.006	−2.630±0.007
0.25	−2.476 231	−2.464 297		
0.375	−2.104 224	−2.100 447		
0.5	−1.778 656	−1.777 177		
0.6	−1.540 288	−1.539 533	−1.526±0.015	−1.542±0.008
1	−0.714 967	−0.714 890	−0.731±0.009	−0.706±0.006

trapped, i.e., localized; in this approximation, the hole has to retrace its path in order to remove the string left behind. However according to Trugman,[7] the hole can propagate across the diagonal of the plaquette without introducing any frustration in the Néel background provided that the hole first makes a loop around the plaquette. It is clear that this involves, for intermediate J_z (1–5), an energy barrier which leads to an exponentially small bandwidth $W \sim a \exp(-bJ_z^{1/2})$, as predicted in the continuum approximation[4] and in the $1/z$ expansion scheme.[15] The bandwidth is here numerically computed by diagonalizing the Hamiltonian in every sector of the momentum **k** and by taking the difference between the highest and the lowest GS eigenvalues. We found that the top of the band is located at $(\pi,0)$ when this wave vector belongs to the reciprocal lattice (for $N=4p$, p integer), or at the closest allowed **k** point. Since, as stated above, the GS momentum is $\mathbf{Q}=\mathbf{0}$ this is indeed the dispersion expected for an effective hopping along the diagonals of the plaquettes. Moreover, we also found that the energies at **k** and $\mathbf{k}+\mathbf{Q}_0$ are quasidegenerate with an accuracy better than 5×10^{-3} of the bandwidth down to $J_z=0.1$ for $N=26$ $[\mathbf{Q}_0=(\pi,\pi)]$. Since this degeneracy is, of course, exact for true antiferromagnetic long-range order (LRO) (because of the doubling of the unit cell), this indicates that, in our largest clusters, the hole almost behaves as if the system were infinite. In other words, the cluster size appears to be sufficiently large in comparison with the extension of a hole wave function, at least for values of J_z that are not too small: this explains the relatively rapid convergence of the GS energies. Note that in order to be able to interpret the one-hole GS momentum **k** as a *quasiparticle* state the latter has to have the same symmetry as the one-hole Bloch state $\tilde{c}_{\mathbf{k},\sigma}\,|\text{Néel}\rangle$.[16] This is indeed the case, as we checked explicitly. For example, the $\mathbf{Q}=\mathbf{0}$ or $\mathbf{Q}=\mathbf{Q}_0$ GS are fully symmetric under 90° rotations as they should be. The behavior of the bandwidth W is shown in Fig. 4. For large J_z, as seen in Fig. 4(b), an approximate exponential decrease with $\sqrt{J_z}$ is seen in agreement with other work.[4,15] The data for $N=16$ and $N=20$ are remarkably close but we observe a systematic deviation for $N=26$. This is attributed to the fact that $(\pi,0)$ does not belong to the reciprocal lattice of the 26-site cluster so that the band maximum lies instead at the closest momentum available. Therefore we believe that the data for $N=20$ are the more accurate for $J_z>0.5$. For smaller J_z the bandwidth remains strongly size dependent although it seems to decrease monotonically with increasing N. We then speculate that $W<0.14t$ (for all J_z) in the thermodynamic limit. This is clearly much smaller than the value of $8t$ that one expects in 2D for a free particle.

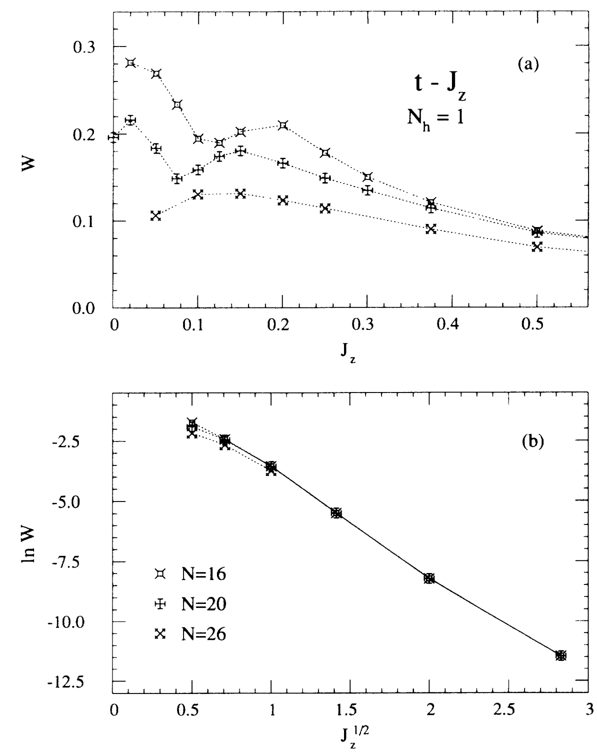

FIG. 4. (a) Bandwidth of one hole in a Néel configuration vs J_z for various cluster sizes. (b) Logarithm of the bandwidth vs $\sqrt{J_z}$ for various cluster sizes.

We now turn to the isotropic limit $J_\perp=J_z=J$. *A priori* the string picture loses here its relevance since the string created along the path of the hole can be cleaned up by quantum fluctuations (term $J_\perp$ in the Hamiltonian). However, for $t>J$, the spin fluctuations can be seen as slow degrees of freedom and the previous arguments of the Ising limit could still be valid here on a time scale smaller than the characteristic time $1/J$ of the spin fluctuations. $J_\perp$ could then be considered as a perturbation.[5,15]

The one-hole GS energy versus J/t is shown in Fig. 2(b) and some related data are listed in Table II. Most of the features seen for the smallest sizes[17,18,9,8] are also ob-

TABLE II. Hole GS energy in the t-J model for several values of J and system sizes $N=16,18,20,26$.

J	$N=16$	$N=18$	$N=20$	$N=26$
0.05			−2.997 176	−2.966 758
0.1	−2.645 011	−2.794 854	−2.777 383	−2.776 582
0.2	−2.298 404	−2.414 355	−2.424 990	−2.418 817
0.25	−2.143 507	−2.253 605	−2.267 583	−2.262 384
0.375	−1.788 890	−1.884 606	−1.908 090	−1.909 901
0.5	−1.466 290	−1.549 693	−1.582 553	−1.593 796

TABLE III. Hole GS energy for the 26-site cluster of the t-J model in the various **k** sector.

J	(0,0)	(π,π)	$\left[\frac{5\pi}{13},\frac{\pi}{13}\right]$	$\left[\frac{10\pi}{13},\frac{2\pi}{13}\right]$	$\left[\frac{4\pi}{13},\frac{6\pi}{13}\right]$	$\left[\frac{9\pi}{13},\frac{7\pi}{13}\right]$	$\left[\frac{3\pi}{13},\frac{11\pi}{13}\right]$	$\left[\frac{8\pi}{13},\frac{12\pi}{13}\right]$
0.1	−2.671 14	−2.682 99	−2.709 43		−2.776 58	−2.732 69		−2.679 52
0.25	−1.935 57	−1.944 92	2.075 57	−2.219 67	−2.262 38	−2.179 41	−2.215 11	−2.003 55

tained in the case of the 20- and 26-site clusters. In particular, the transition to the Nagaoka ferromagnet appears abruptly at small J. However, the small critical value of J that characterizes this transition decreases monotonically with increasing system size. It is then very plausible that the Nagaoka regime will be restricted to the single point $J=0$ in the thermodynamic limit for a vanishing hole density. For J not too small the GS has spin $\frac{1}{2}$ and its wave vector corresponds to the closest momentum to $(\pi/2,\pi/2)$ which is consistent with the periodicity of the BC. With increasing system size the GS momentum jumps discontinously from **k** points to **k** points that are closer and closer (and sometimes equal) to $(\pi/2,\pi/2)$, which is the expected momentum of a single hole in a Heisenberg antiferromagnet. These discontinuities certainly prevent a simple scaling law for the GS energy. However, as seen from Fig. 2 or Table II, the convergence seems to be reasonably fast with some oscillatory behavior for small J. Note that in the definition of ϵ_h, the total energy of the Heisenberg model with N sites (calculated separately) has been subtracted. Unlike the Ising limit, the doubling of the zone (momentum **k** and $\mathbf{k}+\mathbf{Q}_0$ degenerate) is not in general very effective unless N and J are sufficiently large. This means that rather large clusters are indeed necessary to mimic true LRO. However, the rapid convergence of the GS energies may indicate that the hole is in fact more sensitive to the spin correlations at short distances.

Since the convergence for $0.05<J<0.5$ is rather good, we can consider that, in this range, the data for $N=26$ offer a good estimate for the exact GS energy in the thermodynamic limit. It turns out that a fit like (4) indeed works very well providing that

$$\begin{aligned} &\nu \sim 0.685(6)\ , \\ &\beta \sim -3.361(3)\ , \\ &\delta \sim 2.842(8)\ . \end{aligned} \tag{6}$$

This fit gives a lower energy β than previous fits performed for $N=16$ (Refs. 9 and 10) (around -3.18). However the exponent ν is similar and close to $\frac{2}{3}$ as in the Ising limit. The parameters (6) are in good agreement with the prediction of the retraceable path approximation[11] (even better than for the $N=16$ data). This supports the picture that the spin fluctuations are slow degrees of freedom and the string behind the hole survives on a time scale of $1/J$ as mentioned in Ref. 10 which gave the first indications that the string picture could survive the Heisenberg limit.

Although as far as the GS energy behavior is concerned, the Ising and isotropic limits seem very similar, the mechanisms for the coherent propagation of the hole are not. While for the Ising case the hole fills a potential barrier, in the isotropic case it can move quite freely despite its large effective mass dressed by spin fluctuations. For the spin rotationally invariant model one then expects a bandwidth proportional to J as was confirmed by early numerical studies.[8,10,19] The calculation of the bandwidth is, however, subtle since the GS in a given sector of the momentum **k** cannot always be identified with a real quasiparticle state. Indeed, the GS may have a spin $S=\frac{3}{2}$ instead of $S=\frac{1}{2}$ or may not belong to the most symmetric irreducible representation as expected (for examples and details on symmetry classification, see Ref. 9). For completeness we show in Table III the GS energies in the various **k** sectors of the momentum. For both momenta $\mathbf{k}=0$ or $\mathbf{k}=\mathbf{Q}_0$ the GS belongs to the B_1 symmetry of the C_4 group, i.e., it is odd under a 90° rotation (d wave). This clearly means that these states cannot be considered as true quasiparticle states (in fact, they are orthogonal to the Bloch state $\tilde{c}_{\mathbf{k},\sigma}|\text{Heis}\rangle$). Owing to these difficulties the calculation of the bandwidth is left for a future study.

We finish this paper by a remark about the significance of this work. We stress that the GS energy behavior close to $J^{2/3}$ reported first in earlier numerical calculations and confirmed in this paper is, by no means, a definite proof of the string picture. Indeed, only a finite-size scaling of the one-hole spectral function will actually tell whether the agreement with the string picture is only restricted to the GS energy behavior or extends to the excited states.

In conclusion, performing ED on clusters of the t-J model up to 26 sites with a single hole, we found a good convergence of the ground-state energies particularly in the Ising limit where for our largest systems our results indicate exponentially fast convergence. Accurate fits of the energy dependences (with J or J_z) are in good agreement with various analytic approaches based on Brinkman-Rice types of calculations and previous numerical work on small clusters.[8,10,19] In the Ising limit, in light of our data we speculate that the bandwidth is, in any case, smaller than $0.14t$. This work is the first successful test of finite-size scaling approaches in the case of 2D spin-fermion models. It is clear here that a similar analysis can be extended to the extrapolation of excited state properties (such as the much discussed quasiparticle weight factor $z_{\mathbf{k}}$). This is left for future work.

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[11]According to Ref. 10 Eq. (2) has to be changed into $\epsilon_h = -3.34 + 2.93 J^{2/3}$ in the isotropic case. This is obtained by solving the 1D confining problem with some estimates of the nearest-neighbor and second-nearest-neighbor spin correlations of the Heisenberg Hamiltonian.
[12]For $N = 16$ and 18 the point group of the cluster is C_{4v}, i.e., it also includes the reflections with respect to the crystal axes (since in that case $\mathbf{T}_1$ and $\mathbf{T}_2$ are globally unchanged under these operations). For symmetry analysis see, for example, Ref. 9.
[13]The energy of the fully polarized ferromagnet $S_z = (N-1)/2$ is $-4 + NJ_z$ and indeed larger than the GS energy.
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