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New results for the t–J model in ladders: changes in the spin liquid state with applied magnetic field; implications for the cuprates

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Abstract
Exact diagonalization calculations are presented for the t–J model in the presence of a uniform magnetic field. Results for $2 \times L$ ladders ($L = 8, 10, 12$) and 4×4 square clusters with one and two holes indicate that the diamagnetic response to a perpendicular magnetic field tends to induce a spin liquid state in the spin background. The zero-field spin liquid state of a two-leg ladder is reinforced by the magnetic field: a considerable increase of rung antiferromagnetic correlations is observed for J/t up to 0.6, for one and two holes. Pair breaking is also clearly observed in the ladders and seems to be associated in part with changes promoted by the field in the spin correlations around the zero-field pair. In the 4×4 cluster, the numerical results seem to indicate that the field-induced spin liquid state competes with the zero-field antiferromagnetic short range order, the spin liquid state being favoured by higher doping and smaller values of J/t. It is interesting to note that the field effect can also be observed in a 2×2 plaquette with one and two holes. This opens up the possibility of gaining a qualitative understanding of the effect.

1. Introduction

The long-standing problem of understanding the dynamics of a charge carrier in an antiferromagnetic (AF) background [1] is at the centre of the high T_c puzzle. For example, one of the important controversies still not settled is deciding whether a hole injected into an AF Mott insulator will keep its integrity [2] or dissociate [3]. These options imply two completely different ways of looking at the corresponding ground states: the first is as a Fermi liquid and the second is not. In the first case, does the spin–polaron concept [2] capture all the basic ingredients of charge carrier dynamics in the cuprates? In the second, does the resonating valence bond state [3], and the associated idea of spin–charge separation, lead to an understanding of the phases at higher doping? In addition, recent numerical results for the Hubbard model [4], consistent with optical measurements [5], have raised the possibility of a *partial* spin–charge separation. The lack of an exact solution, either analytic or numerical, for strongly correlated models for the cuprates, like the t–J or Hubbard models, is at the origin of this and other controversies. It has been realized for some time already that in addition to the technical difficulties associated with solving the most common model Hamiltonians for the cuprates, the fact that all these models seem to have a variety of competing ground states with different order parameters makes it even more difficult to obtain a clear picture. This multiplicity of competing ground states is reflected in the richness of the cuprate phase diagram and has given high visibility to theories which explore quantum phase transition (QPT) ideas [6]. In some cases, this competition seems to be resolved through the mutual coexistence of two different order parameters, as in the specific case of the stripes observed through neutron scattering measurements [7],[3] or the recurrent observation of AF order in the superconducting (SC) phase [9] through nuclear magnetic resonance (NMR), and muon spin rotation (μ-SR). It is important to notice that parts of the various aspects revealed by experiments emerge in results obtained with different methods applied to slightly different Hamiltonians; however the overall picture never seems complete or coherent. Until a theoretical breakthrough occurs, with the appearance of some new analytical or numerical method which can finally settle these issues, researchers in this field will keep an attentive eye on new experimental results which can provide some clue about the true nature of the dynamics of charge carriers in an AF background.

In this respect, a recent experimental development has renewed interest in this subject: neutron scattering [10][4], scanning tunnelling microscopy (STM) [11][5], and NMR [12] experiments have shown that the application of an external magnetic field can change the relative presence of two of the most fundamental order parameters in the cuprates: AF and SC order parameters. The presence of the first is enhanced at the expense of that of the second. Apparently, extensive regions of AF order (centred in the vortex cores) were observed to develop as the strength of the magnetic field increases. This seems to be true for different materials (YBCO, LSCO and BSSCO) at different doping concentrations[6]. Although a complete experimental picture has not yet emerged, the neutron scattering experiments on optimally doped LSCO, for example, have indicated a substantial increase of inelastic scattering intensity at low energy transfers with increasing magnetic field (see footnote 4). This seems to imply that the field induces slowly fluctuating AF spin correlations. However, several questions still remain: Is this effect generic to all cuprate families at all dopings? In what circumstances is the field-induced magnetism static and when is it dynamic? And very importantly, is the field-induced AF magnetism restricted to the vortex cores or is it present everywhere in the system?

$SO(5)$ theories [14] had predicted the possibility of antiferromagnetism inside the vortex cores in cuprates [15]. The qualitative idea is that once superconductivity is suppressed, either by impurities or magnetic field, AF order should be enhanced. In addition, after the above-mentioned experiments, mean-field calculations using effective Hubbard-like Hamiltonians

[3] For a recent review of the mapping of incommensurate spin fluctuations in LSCO through neutron scattering, please see [8].
[4] A comprehensive review of the neutron scattering results at finite magnetic field can be found in [8].
[5] Note that STM is not sensitive to the magnetic moments. The assumption here is that the charge density wave observed in and around the vortices is associated with incommensurate AF spin order, like in the stripes observed by means of neutron scattering [7].
[6] Some recent μ-SR experiments have apparently challenged some of the conclusions obtained by neutron and STM experiments. Please see [13].

produced results in agreement with this qualitative idea [16]. This however comes as no surprise, since these effective Hamiltonians already include explicitly a term for pairing and an on-site Coulomb repulsion, which favours AF order. For these mean-field calculations, one expects the suppression of one order to automatically lead to the enhancement of the other. QPT theories, on the other hand, state that the above experiments are an indication that the superconducting phase is in the vicinity of a bulk QPT to a state with microscopic coexistence of superconducting and spin density wave orders [17]. It is also claimed that the STM results showing the appearance of charge density wave order can be accounted for by QPT-type theories [18].

Two of the most popular models for the cuprates are the t–J and Hubbard models. Much of what is known about how charge carriers move in an AF two-dimensional (2D) background was obtained through their analysis. Prominent among the methods used for this are numerical techniques [19]. However, to the best of our knowledge, no non-mean-field calculations of a strongly correlated Hamiltonian (Hubbard- or t–J-like) have been performed to analyse the effect of an external magnetic field upon the spin correlations. Previous numerical results for small square clusters were concentrated on the issues of spin–charge separation [20] and magnetic susceptibility of the ground state [21], but neither work analysed the evolution of spin–spin correlations with the external magnetic field. Unfortunately, these two works attracted very little attention. One of the reasons may have been the fact that they were published before the main experimental results showing the effect of the magnetic field were performed. Another factor is the difficulty, mainly after introducing the magnetic field, of performing finite-size scaling analysis for square clusters, a necessary step in ascertaining any claims based on the numerical results [21]. There is however an alternative route in obtaining credible numerical results which can extend these two previous works, and provide some clues about the overall problem of charge carrier dynamics in an AF background: performing the calculations in $2 \times L$ ladders. For some time already, two-leg ladders have been a fruitful testing ground for the numerical study of strongly correlated models relevant to the cuprates [22]. This is especially true for exact diagonalization (ED) calculations, where the quasi-unidimensional aspect of ladders makes feasible the study of finite-size effects, providing credibility to the results[7]. Besides that, given the above-mentioned difficulty in extracting uncontroversial conclusions from numerical results obtained for square clusters (with either ED or density matrix renormalization group (DMRG) [24] methods), some of the more solid numerical results obtained for two-leg ladders have been qualitatively 'translated' into the 2D cuprate arena [25, 26].

In this paper, the authors present zero-temperature ED calculations for the t–J model with a magnetic field in hole-doped two-leg ladders. All the calculations for ladders were done adopting periodic boundary conditions (PBC) along the legs. The results show that the diamagnetic response of the system leads to a strengthening of the rung spin correlations. This can be described in qualitative terms as a reinforcement of the spin liquid (SL) character of the two-leg ladder ground state. In light of our conclusions for two-leg ladders, and in keeping with the spirit of the discussion in the previous paragraph, the authors also performed calculations on small square clusters. The ED results for 4×4 clusters presented intriguing results: the calculation of spin correlations for different values of J/t, different dopings (one and two holes) and using different boundary conditions (PBC and open boundary conditions (OBC)) seem to indicate that the movement of the holes, under the influence of the external field, promotes the appearance of an SL state in the spin background. This is consistent with the results for ladders; however, in the square clusters this SL state has to compete with the

[7] A brief list of recent ED results for two-leg ladders includes the following references: [23].

zero-field AF short range order (SRO) characteristic of doped cuprates. Although the results are not conclusive[8], they point to a possible new example of competition between different ground states in a strongly correlated model related to the cuprates [6]. The rest of the paper is organized as follows. In the next section, a brief description of the Peierls transformation is given. Then, in section 3, results are presented for two-leg ladders, followed by results for a 4×4 cluster. A summary, conclusions and prospects for future work are presented in the last section.

2. Adding the field to the t–J Hamiltonian: the Peierls transformation

The magnetic field is introduced in the t–J model through a Peierls transformation:

$$H = J \sum_{\langle ij \rangle} [\mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{1}{4} n_i n_j] - t \sum_{\langle ij \rangle \sigma} [c^\dagger_{i\sigma} c_{j\sigma} \exp(\mathrm{i}\theta_{ij}) + \mathrm{h.c.}], \tag{1}$$

where $c_{i\sigma}$ is a fermionic annihilation operator with doubly occupied states projected out, $\langle\,\rangle$ indicates that the summations include only nearest-neighbour (NN) sites and σ stands for the spin degree of freedom. The phase in the hopping term can be written, using a Landau gauge $\mathbf{A} = B(0, x, 0)$, as

$$\theta_{ij} = \frac{e}{h} \mathbf{r}_{ij} \cdot \mathbf{A}(\mathbf{r_i}), \tag{2}$$

and the magnetic field B is related to the dimensionless flux per plaquette through $\alpha = 2\pi B a_0^2/\phi_0$, where ϕ_0 is the unit flux quantum and a_0 is the lattice parameter[9]. It is important to remark that, as one of the main objectives of the present work is to gain insight into the dynamics of charge carriers introduced into an AF background, the calculations concentrate in the diamagnetic response of the charge carriers to the external field, and will therefore omit the Zeeman term. For laboratory-strength magnetic fields, this can be considered a reasonable approximation to the actual experimental situation. However, for the calculations presented here, mainly for square clusters, where the fields involved can be quite substantial[10], the Zeeman term would have to be taken in account if one wished to make any connection to the experimental results mentioned above [10–12].

3. Results for two-leg ladders

3.1. Single-hole results

As is well known [28], the spin sector in ladders is gapped and therefore presents the exponential decay of AF spin correlations in the leg direction, characteristic of a SL state. In a qualitative sense, the SL character of the undoped ground state in ladders can be described as a collection of rung singlets [28]. This picture survives doping with holes up to a moderate concentration [29]. Therefore, to obtain a qualitative understanding of how the magnetic field affects the zero-field ground state, correlations between spins in the same rung (from now on called rung correlations) were calculated as a function of field. In figure 1(a) we show the evolution with field (in terms of α) of the rung correlations in a 2×8 ladder with one hole, for $J/t = 0.2$, 0.4 and 0.6. It can be seen that there is a substantial increase of the rung correlations, while correlations for spins

[8] Efforts are being made by the authors to extend the calculations to considerably larger square clusters.
[9] Adopting PBC in the 4×4 cluster leads to the quantization of the magnetic flux (see [27]). The same does not happen for ladders; however, the results for ladders will also be presented for discrete values of the parameter α.
[10] For one flux quantum threading each plaquette in the 4×4 cluster, the order of magnitude of the associated field is 1 kT.

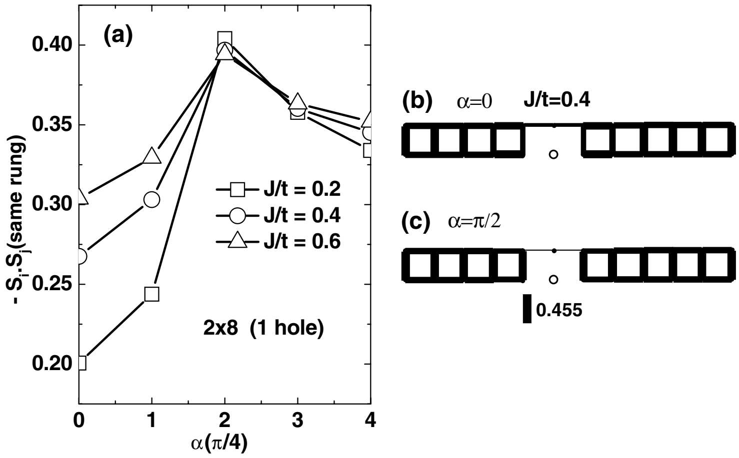

Figure 1. (a) Variation with field of rung spin correlations for a 2×8 ladder with one hole, for $J/t = 0.2, 0.4$ and 0.6. Note the substantial increase of the rung correlations as a function of magnetic field, especially for lower values of J/t. ((b), (c)) 2×12 calculations for $J/t = 0.4$ and one hole. Representation of the NN spin correlations after projecting the hole (open circle), for zero field (b) and $\alpha = \pi/2$ (c). The thickness of the lines is proportional to the absolute value of the correlations. All values are negative (AF). In (b), note the weakening of the AF spin correlations in the rungs close to the projected hole. In (c), note how the rungs close to the hole have their AF spin correlations increased, compared to the zero-field case in (b), especially the ones adjacent to the projected hole. The line at the bottom of (c) represents the rung correlation for an *undoped* 2×12 ladder.

further apart than $d = \sqrt{2}$ are always smaller than the zero-field value (see below). As the magnetic field influence on the spin background is being assessed through the hole movement, one would expect a more pronounced effect at lower values of J/t, when the hole has higher mobility and is more effective in driving the behaviour of the spin background. As can be observed by comparing results for $\alpha = 0$ and $\pi/4$, the increase of the spin correlations is larger for smaller values of J/t. However, a substantial increase is still present for $J/t = 0.6$.

It is interesting to take a closer look at how the spin correlations around the hole will change with the magnetic field. To do that, one can project out of the ground state wavefunction all the states where the hole occupies one specific site and use these states to calculate the spin correlations. Figures 1(b) and (c) compare the results for $\alpha = 0$ and $\pi/2$ in a 2×12 ladder with one hole, for $J/t = 0.4$. The thickness of the lines is proportional to the absolute value of the correlations (all correlations displayed are AF). For zero field (figure 1(b)) one can see the distortion in the spin background caused by the presence of the hole (open circle in the figure): the rungs adjacent to the hole have their spin correlations substantially decreased, in comparison with rungs far away from it, which display correlations similar to the ones in the rungs of undoped ladders. For smaller values of J/t the distortion of the spin background extends to larger distances, consistent with the higher mobility of the hole[11]. The application of the magnetic field, as can be seen in figure 1(c), affects drastically the zero-field spin background: all rungs close to the projected hole have their AF spin correlations enhanced,

[11] Calculations at zero field [30] have indicated that as J/t decreases there is a tendency of the one-hole ground state in $2 \times L$ ladders to gradually move to sectors of higher total spin. This indicates the ability of the hole to influence ever larger regions of the spin background as its mobility increases, changing even the qualitative character of the ground state. See Muller and Rice [30] for discussions of ferromagnetism in doped ladders.

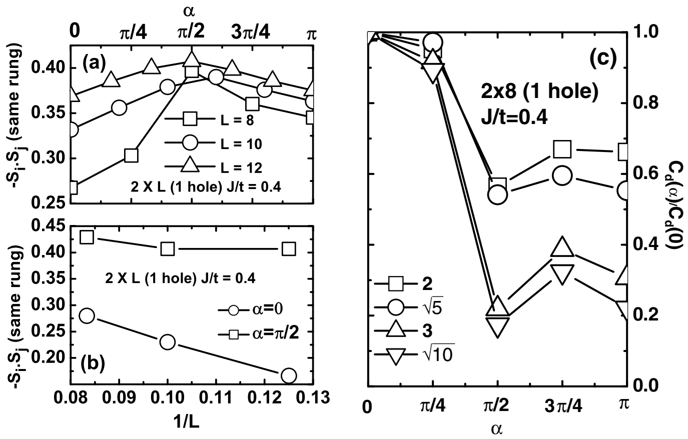

Figure 2. (a) Analysis of the evolution with magnetic field of the rung correlations for ladders of increasing length. Results are shown for $2 \times L$ ladders ($L = 8, 10, 12$) with one hole, $J/t = 0.4$. (b) Variation with $1/L$ of the rung spin correlation for $2 \times L$ ladders ($L = 8, 10, 12$) with one hole and $J/t = 0.4$. The spin correlation shown is for the rung adjacent to the projected hole. Results are shown for zero field (circles) and $\alpha = \pi/2$ (squares). Note that the finite-field results are considerably less dependent on L than the zero-field results (see the text). (c) Dependence on field of long distance spin correlations in ladders: the ratio between the correlations at finite field and zero field for different distances. Note the sharp decrease of the ratio (at all distances) as the field increases. C_d is defined as $\vec{S}_i \cdot \vec{S}_{i+d}$.

particularly the ones adjacent to the hole, when compared to the zero-field values[12]. One can describe the new spin arrangement as a set of 'strong rung singlets'. As a reference, we show at the bottom of figure 1(c) a line which is representative of the rung correlations of an *undoped* 2×12 ladder, showing that some of the rung correlations for $\alpha = \pi/2$ are even larger than in the undoped system. Similar calculations for smaller ladders ($L = 8, 10$) produce very similar results, indicating that any size effects present are small and do not affect the qualitative description of the results.

Regarding size effects, one should note that, at zero field for $J/t = 0.4$ (figure 1(b)), rungs as far as three lattice spacings away from the projected hole are affected, having their spin correlations *decreased* as compared to the undoped ladder case. The fact that this differs very little from 2×10 results indicates that at zero field the results are quite well converged for a 2×12 ladder. At finite field (figure 1(c)), the distortion caused by the field, i.e., the *increase* in the rung correlations when compared to the zero-field results, has approximately the same reach (three lattice spacings from the projected hole), indicating that the results seem well converged also with field for a 2×12 ladder. Now, results are presented for different ladder sizes. In figure 2(a) it is shown how the rung correlations evolve for increasing ladder sizes ($L = 8$, 10 and 12) in the single-hole case. Although the comparison is not intended as a true finite-size scaling analysis, since the hole doping decreases from 1/16 to 1/24, it indicates that the magnetic field effect does not seem to vanish as L increases. As discussed already in connection with figure 1(c), the $J/t = 0.4$ single-hole calculations in a 2×12 ladder are already representative of qualitative bulk behaviour at low doping. It would be interesting though to extend the calculations performed here by using other methods (for example, DMRG ones) and also by performing ED calculations with twisted boundary conditions [31]. Another way

[12] It is interesting to note that the increase in the spin correlations of the rungs adjacent to the hole seems to be responsible for the substantial decrease in the spin correlations of the bonds in the leg opposite to the projected hole.

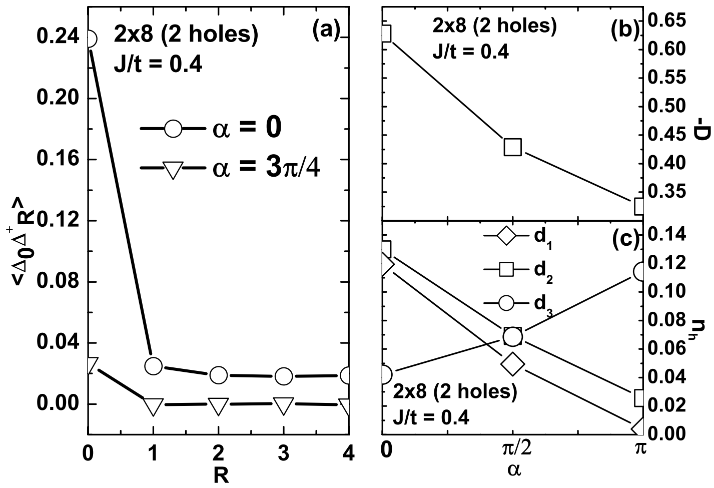

Figure 3. (a) Pair–pair correlations for a 2×8 ladder with two holes for $J/t = 0.4$ at zero (circles) and finite field (triangles). (b) Variation with field of spin correlations across a $\sqrt{2}$ diagonal when the two holes are projected in the other diagonal of the same plaquette (for the same cluster and parameters as in (a)). (c) Field variation of the probabilities for three different hole configurations: holes sitting at the same rung ($d_1 = 1$, diamonds); holes in the diagonal of a plaquette ($d_2 = \sqrt{2}$, squares) and holes at maximum distance ($d_3 = \sqrt{17}$, circles). The second configuration is the most probable at zero field ($\alpha = 0$) and the third is the most probable for $\alpha = \pi$ (same cluster and parameters as in (a) and (b)).

of probing the magnetic field effect is to check how the 'projected hole' spin correlations (as displayed in figures 1(b) and (c)) change with L. Figure 2(b) shows how rung spin correlations vary with L for the rung adjacent to the projected hole. Results are shown for $2 \times L$ ladders ($L = 8, 10, 12$) with one hole and $J/t = 0.4$, for zero field (circles) and finite field ($\alpha = \pi/2$, squares). The variation with $1/L$ at finite field is considerably less than at zero field (notice that the hole concentration is *not* constant; it varies from $n_{\text{h}} = 0.0625$ to $n_{\text{h}} \approx 0.0417$). The smaller variation with ladder size at finite field seems to indicate the *local* character of the field effect. This is in agreement with results (to be discussed below) which indicate that the field effect is present even in a small 2×2 cluster with one and two holes.

To complete the analysis, calculations were done for longer range spin correlations. One would expect the increase of the rung correlations to lead to an overall decrease of the spin correlations along the legs (in the limit where the rungs form perfect singlets, the spins would be completely uncorrelated along the legs). In figure 2(c), we show the field dependence of long distance spin correlations in a 2×8 ladder with one hole for $J/t = 0.4$. The decrease with field of the ratio between finite- and zero-field correlations for all distances larger than $\sqrt{2}$ is consistent with an increase in the SL character of the ground state at finite field[13].

3.2. Adding a second hole: pair breaking with applied field

It is interesting to note that a second hole added to the system depicted in figure 1(c) will not tend to form a pair with the first one. In reality, they tend to stay as far as possible from each other and a calculation of spin correlations shows that the 'strong rung singlets' picture still holds. In figure 3(a), results are shown for pair–pair correlations at zero and finite field for

[13] The decrease of the $\sqrt{2}$ correlation with field occurs only at higher values of the field (for $\alpha > \pi/2$ at $J/t = 0.4$ with one hole).

a 2×8 ladder with two holes and $J/t = 0.4$. The pair operators are defined as singlet pair operators in the rungs: $\Delta = (c_{i+}c_{j-} - c_{i-}c_{j+})$, where i and j are two sites in the same rung (for details, see [26]). The results clearly show the pair-breaking effect of the magnetic field, as well as the loss of coherence in the pair propagation along the ladder. Our calculations also indicate that the presence of the magnetic field makes it energetically favourable for the pair to break and for the spin background to form strong rung singlets, in contrast to the zero-field case, where the preferred configuration is the formation of a bound pair, where the holes are separated by $\sqrt{2}$ with a strong *across-the-diagonal* AF spin correlation [25]. Figure 3(b) shows the variation with field of the across-the-diagonal spin correlation (denoted as **D**) for a 2×8 ladder with two holes and $J/t = 0.4$. The suppression of the across-the-diagonal correlation by the field partially explains the pair-breaking effect. Compared to that for $\alpha = 0$, the value of **D** for $\alpha = \pi$ has decreased to half. This is accompanied by an increase in the average separation of the two holes. In figure 3(c) (again for 2×8, two holes, $J/t = 0.4$), after one hole is projected at an arbitrary site, results are shown for the density n_{h} of the second hole at three different distances from the projected hole. Diamonds indicate the probability of two holes occupying the same rung (second most probable configuration at zero field, with $d_1 = 1$). Notice how this probability decreases very markedly with applied field, becoming negligible for $\alpha = \pi$. The squares indicate results for distance $d_2 = \sqrt{2}$ (the most probable hole configuration at zero field) and the circles for $d_3 = \sqrt{17}$ (the most probable hole configuration at high field). At this point, the following observation is appropriate: at first sight, it appears counterintuitive that at finite field the pair will be broken. After all, the single-hole results above have shown that the field has increased the overall strength of the rung correlations. And, using an argument based on the optimization of the ground state energy, it seems reasonable that the second hole would pair up with the first one in the same rung, thus minimizing the number of broken AF bonds in the rungs. However, as was shown in the (zero-field) numerical work of White and Scalapino [25], the structure of the pair is more complicated. It is not only the magnetic energy that has to be optimized; the kinetic energy of the two holes has to be taken in account also: their ability to hop from a $\sqrt{2}$ configuration (when they are positioned in the diagonal of a plaquette) to a minimum distance configuration (positioned in one of the rungs of the same plaquette) is more important than just minimizing the number of broken AF bonds in the rungs. One piece of evidence is the fact that (for values of J/t around 0.4) the $\sqrt{2}$ configuration for the holes is more probable than a same-rung configuration. And, as found by White and Scalapino [25], the matrix element of the hopping term connecting these two configurations is critically dependent on the existence of a strong AF bond in the opposite diagonal to the diagonal occupied by the holes when they are in the $\sqrt{2}$ configuration. One has therefore the picture at zero field of a pair of holes 'straddling' the AF bond formed in one of the diagonals of a plaquette. Our results in figure 3(b) indicate that the presence of the field weakens considerably this 'across-the-diagonal' spin configuration, leading to the 'ungluing' of the pair. This break-up of the pair is shown in figure 3(c) as the simultaneous decrease with field of the probabilities for the configurations d_1 and d_2.

4. Results for a 4×4 cluster

4.1. NN correlations for one and two holes

Motivated by the interesting results obtained for ladders, the authors also performed calculations for the t–J model in 4×4 clusters with one and two holes. As already mentioned above, extreme caution has to be exercised in interpreting the results. However, the authors believe the interpretation of the ladder results can help our intuition in understanding the

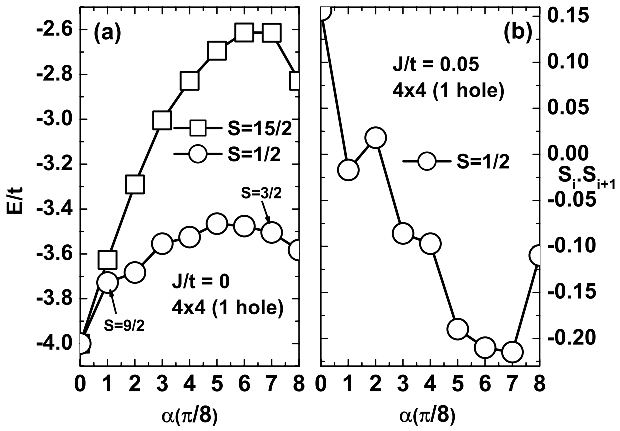

Figure 4. (a) Variation of energy with magnetic field in a 4×4 cluster with one hole for $J/t = 0$. Squares: ground state energy for the $S = 15/2$ sector. Circles: absolute ground state energy. $S = 1/2$ for all values of α, with the exception of $\alpha = \pi/8$ ($S = 9/2$) and $7\pi/8$ ($S = 3/2$). (b) Variation of NN spin correlations with magnetic field for a 4×4 cluster with one hole for $J/t = 0.05$. The field drives the system from a ferromagnetic state to a new state with AF NN spin correlations.

4×4 results. In an attempt to bolster the confidence in the results obtained, calculations were performed using PBC and OBC. For reasons which will become clear soon, we start the calculations for the 4×4 cluster with values of $J/t < 0.1$. In figure 4(a), results for the energy variation with magnetic field are shown for $J/t = 0$ in a 4×4 cluster with one hole. The squares are results for the totally polarized $S = 15/2$ sector and the circles are results for the *absolute* ground state sector. For $J/t = 0$, at zero field, as is well known, the ground state of the t–J model with one hole is totally polarized ($S = 15/2$, for this case) [32]. However, at low field (as seen in figure 4(a)), with just one flux quantum threading the cluster ($\alpha = \pi/8$), the polarization of the absolute ground state is already below saturation ($S = 9/2$), and for all other values of α the total spin of the ground state is $S = 1/2$, with the exception of $\alpha = 7\pi/8$, where $S = 3/2$. As noted in Veberič *et al*[14], the field dependence of the energy for the $S = 15/2$ sector (squares in figure 4(a)) is expected, as a consequence of the increase of the hole energy with the cyclotron frequency: $\delta E_{\rm h} = eB/m_{\rm eff}$ (however, see [33]). On the other hand, to the best of our knowledge, the change of the ground state sector from fully polarized at zero field to $S = 1/2$ at finite field was never discussed. It is natural to expect that, whatever the effect introduced by the magnetic field, the lowering of the total spin of the ground state to its minimum value should be associated with the development of AF correlations. To test this hypothesis, NN spin correlations in the $S = 1/2$ sector were calculated for $J/t = 0.05$ with one hole in a 4×4 cluster[15]. The results are presented in figure 4(b), where it is shown that the magnetic field initially turns the ferromagnetic NN spin correlations into AF correlations and gradually enhances them. Similar results are obtained for $J/t = 0$, indicating that it is not the gain in magnetic energy which drives the increase in the NN AF correlations. The results at higher values of J/t are similar to the ones in figure 4(b), *but only up to* $J/t \approx 0.07$. A small increase in the NN AF correlations can be achieved at higher values of field ($\alpha = 7\pi/8$) up to $J/t \approx 0.1$. Therefore, from the single-hole results at small values of J/t it is clear that the

[14] See figure 3 of reference [21].
[15] In a 4×4 cluster with one hole, the total spin of the zero-field ground state is $S = 15/2$ for $J/t < 0.075$. For a recent discussion of the t–J model at low J/t values see [34].

field (when only the diamagnetic response is included in the Hamiltonian) is able to change radically the character of the ground state: from fully polarized to minimum polarization. However, this effect is gradually weakened, until it is no longer present, as J/t increases. It is well known from the early numerical studies and from photoemission measurements [19] that the hole bandwidth is strongly renormalized by J. As mentioned in the ladder discussions above, the size of the region (in the spin background) affected by the hole presence decreases as J/t increases. In the limit where $J/t \gg 1$, an injected hole would be unable to move[16]. As the field effect is caused by the hole movement, it is natural to expect that it will become weaker as the ability of the hole to move is degraded by the stiffening of the spin background with increasing J/t. However, a value of $J/t = 0.1$, although already introducing very short range AF fluctuations in the spin background, still allows the hole a fair amount of freedom for moving around the 4×4 cluster. Therefore, it is puzzling that the effect of the field in the NN correlations is already negligible for $J/t \approx 0.1$. (However, as will be shown later, the effect is more resilient at longer distances.) One possible explanation for the existence of a threshold at $J/t \approx 0.1$ in the field effect is that the hole movement under the influence of the field tries to induce a ground state with a *qualitatively different* spin background to the one at zero field, and this sets in a competition between different ground states. For very small J/t, where the zero-field ground state is the Nagaoka phase [32][17], the new 'order' (imposed by the field and characterized by minimum polarization) quickly dominates. It is well known that the Nagaoka phase is very delicate and that small perturbations are able to drive the system out of it. Therefore, the effect in figure 4(b) is not hard to accept. However, for values of J/t where the 4×4 cluster at zero field has already moved out of the Nagaoka phase, to a more robust ground state, the field is not able to impose its new type of 'order' to all distances. Therefore, if one could somehow 'weaken' the zero-field ground state, the field generated ground state would certainly be still visible at higher values of J/t. One way of weakening the zero-field ground state is to increase the hole concentration.

Figure 5(a) shows the variation with field of NN AF spin correlations in a 4×4 cluster with two holes, for $J/t = 0.2$, using PBC. Contrary to what was observed for the single-hole case, for two holes the increase of NN AF correlations with magnetic field survives up to higher values of J/t (up to ≈ 0.3). This is consistent with the idea that the field effect will be observable at higher J/t values if the zero-field ground state is somehow weakened, since it is well known that in the t–J model the short range order associated with AF fluctuations is weakened at higher hole concentrations. At this point, one is then tempted to suggest, in view of the results for ladders, where the field seems to *reinforce* the SL character of the zero-field ground state, that in the square clusters the field also tries to create a SL state which has characteristics incompatible with those of the zero-field state. This sets up a competition which is regulated by doping and the value of J/t: higher dopings favour the field generated state and higher J/t favours the zero-field state. One can now try to get a better idea of how this competition evolves by looking at spin correlations beyond NN and comparing the results with and without field. However, before doing that, it is important to verify how the results for square clusters depend on the boundary conditions. All the results shown up to this point have been for PBC. Figure 5(b) depicts NN correlations for $J/t = 0.1$ in a 4×4 cluster with two holes at zero field, now using OBC. The thickness of the lines is proportional to the absolute value of the spin correlations between the connected sites (all correlations shown are AF). For comparison, figure 5(c) shows the results at finite field ($\alpha = \pi$). It can be easily seen that the

[16] Obviously, in a real material, phase separation (between hole rich and hole poor regions) sets in before the holes become virtually immobile. For a discussion of numerical results for phase separation in the t–J model, please see [19].

[17] The ferromagnetic state thus created is the so-called Nagaoka phase.

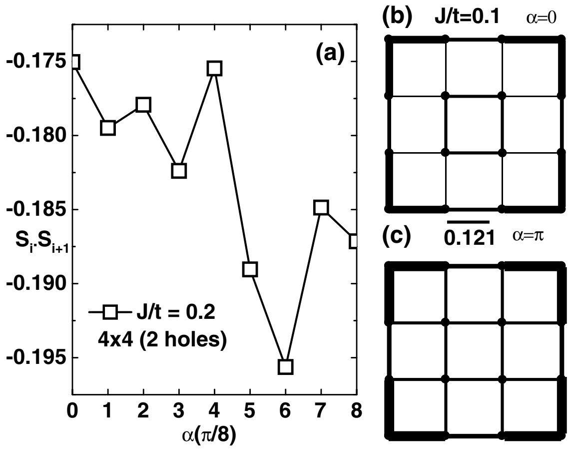

Figure 5. (a) NN spin correlations in a 4×4 cluster with two holes for $J/t = 0.2$. Despite some deviations for $\alpha = \pi/2$ and $7\pi/8$, the overall trend indicates that the magnetic field promotes an increase of the NN AF correlations. ((b), (c)) Representation of the NN spin correlations in a 4×4 cluster (using OBC) with two holes for $J/t = 0.1$ at zero field (b) and $\alpha = \pi$ (c). The thickness of the lines is proportional to the absolute value of the correlations. All values are negative (AF). The line at the top of figure 4(c) serves as a reference. Note the overall increase of NN AF correlations with field. This shows that the results presented here do not depend qualitatively on the boundary conditions used.

field enhances the NN AF spin correlations also for OBC, showing that the effect presented here is not dependent on boundary conditions.

4.2. Effect of field in the longer range spin correlations

4.2.1. Review of zero-field results. Before looking into the effect of the field in the longer range correlations, a discussion will be presented of how the zero-field static magnetic correlations at different dopings are described through ED calculations in a 4×4 cluster. It is our belief that the presentation of a somewhat detailed account of how the zero-field magnetic ground state in the 4×4 cluster evolves with doping from AF long range order (LRO) to AF SRO will clarify the description and interpretation of the finite-field results[18]. In figure 6(a), correlations between spins at different distances are shown for a 4×4 cluster at different dopings at zero field, for $J/t = 0.1$.[19] Squares show spin correlations at zero doping, and diamonds and circles display spin correlations for one and two holes, respectively. It is well known, through calculations using different methods [35], that the Heisenberg model in two dimensions (to which the t–J model at zero doping is equivalent) presents AF LRO at zero temperature (2D Néel order). This *static* order translates, in a plot of spin correlations as a function of distance between spins, into a finite-value plateau at long distances. Because of the limited distances available in a 4×4 cluster, the results in figure 6(a) for zero doping (squares) only display a

[18] As mentioned in the introduction, details of the evolution with doping of the ground state of any strongly correlated model related to the cuprates are not free of controversies and are at the centre of the high T_c problem. Therefore, in the following, we will discuss mainly the more well established results. In what follows, results will be presented only for *static* spin correlations. For a discussion of the *dynamical* aspects of zero-field spin correlations, as well as static incommensurate order, please see [8].
[19] For clarity of presentation, the figure concentrates on the NN correlations and the two largest distances in the 4×4 cluster. These are enough to present the main ideas in the discussion.

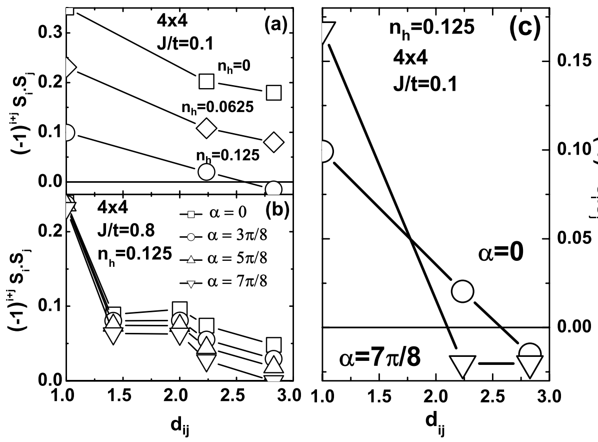

Figure 6. Variation of spin–spin correlations with distance for a 4×4 cluster. Results are shown at zero doping and with one and two holes, at zero and finite field. (a) Results for $J/t = 0.1$ at zero field. Squares: zero doping, showing for a small square cluster how the AF LRO (2D Néel order) is displayed. The tendency of the spin correlations to form a plateau at larger distances is an indication of the AF LRO expected at the thermodynamic limit. Diamonds: results for one hole ($n_h = 0.0625$) indicate the transition from Néel order to AF SRO at finite doping. Although the correlation length is now finite, it is clearly larger than the cluster size. Circles: results for two holes ($n_h = 0.125$) indicate that the NN AF correlation is substantially decreased if compared with the zero-doping case and that the correlations for larger distances are very close to zero (at a distance of $2\sqrt{2}$ the correlation becomes ferromagnetic). This indicates that the correlation length of the AF SRO is of the order of the cluster size. (b) Variation of the spin correlations with distance and field in a 4×4 cluster with two holes and $J/t = 0.8$. The decrease of the correlation length as the field increases can be clearly seen; however the NN correlations are not affected (this is true for $J/t > 0.3$). (c) Comparison of spin correlations for $J/t = 0.1$ with two holes at zero and finite field. Notice that besides decreasing the correlation length, the field also increases markedly the NN AF correlation, in contrast with results for $J/t > 0.3$. This suggests that at low values of J/t the field induces a *qualitatively* different ground state.

tendency to level off and form a plateau[20]. What would then be expected as the 4×4 cluster is doped with the first hole? It is well known from several experimental results [37] that the Néel phase (AF LRO) is destroyed for a hole concentration $n_h \approx 0.02$. Therefore, for a doping of $1/16$ ($n_h = 0.0625$), one would naively expect the spin correlations in the t–J model to display no trace of antiferromagnetism. However, the numerical results seem to indicate otherwise: judging from the curve for $n_h = 0.0625$ (diamonds) in figure 6(a), one would say that there are still quite robust AF tendencies in the doped system. In reality, this is in agreement with experimental results, mainly neutron scattering ones [37, 38], which describe this situation as AF SRO. In the cuprates, an AF exchange interaction between the copper oxide planes leads to three-dimensional (3D) Néel order with a transition temperature $T_N \approx 300$ K (at zero doping). It is this 3D order which quickly fades away at around $n_h = 0.02$ and is represented by a narrow strip close to zero doping in the phase diagram for the cuprates. However, strong AF correlations remain in the copper oxide plane. The energy spectra of these AF correlations

[20] Quantum Monte Carlo (QMC) results for the Hubbard model at zero doping in clusters with up to 64 sites can be seen in figure 14(a) of [19]. The very clear plateau presented there is an indication that the Hubbard model at zero doping (as well as the t–J model at zero doping) captures the essential behaviour of the spin background. QMC results for the t–J model at zero temperature and finite doping, which became available in the last few years (see, for example, [36]), have shown that the t–J model 'overestimates' the AF order, by predicting its survival to higher values of doping than experimentally observed. However, the same technique (see Anisimov [36]) predicts that including longer range hoppings in the t–J model will bring the numerical results into agreement with the experimental data.

(its fluctuations at different frequencies) have a very rich structure and a very complex dependence on doping. In addition, several aspects of the experimental results are not yet settled, different cuprate families presenting different results. However, due to the very strong AF exchange interaction between the copper spins in the planes, it is not totally surprising that AF scattering of some sort is present in neutron experiments at dopings considerably higher than $n_h = 0.02$. This surviving magnetism is generally referred to as AF SRO, and it is thought by many to play a very important role in defining the properties of the cuprates for a wide region of the phase diagram. It can survive to moderate dopings, well into the metallic phase [38]. It is this AF SRO which is displayed by the somewhat robust one-hole spin correlation results (diamonds) in figure 6(a). Early ED results have shown that the t–J model is able to capture this crucial property of the cuprates [39]. When a second hole is introduced into the 4×4 cluster ($n_h = 0.125$) the spin correlations (circles) become ferromagnetic for the longest distance available in the cluster (namely, $2\sqrt{2}$) and are very close to zero for $\sqrt{5}$. This is again in good agreement with neutron scattering results, where the correlation length ξ of the AF SRO decreases with doping n_h approximately as $\xi = 3.8/\sqrt{n_h}$. Not coincidentally, this formula also describes the variation with n_h of the average separation between holes [38]. At moderate doping, ξ can indeed be very short: in the metallic state of LSCO, for $n_h \approx 0.175$, one has that $\xi \approx 10$ Å, which corresponds to approximately two lattice parameters. This is in qualitative agreement with the results for $n_h = 0.125$ (circles) in figure 6(a), since the distance where the correlations turn from AF to ferromagnetic provides an estimate of ξ. This discussion then shows that, despite the small size of the cluster analysed, one can obtain reliable qualitative information, through the t–J model, about some aspects of the magnetism in the ground state of the cuprates.

4.2.2. Field effect: competition between AF SRO and SL? The discussion now turns to examining how *longer range spin correlations* are affected by the field. In the ladder results above, it was shown that spin correlations at larger distances than $\sqrt{2}$ were decreased by the external field (see footnote 13). What are the results for square clusters? Although the authors are currently working on extensions and improvements of the present calculations (see footnote 8), for now a tentative picture can be summarized as follows. As mentioned already, the NN spin correlations increase substantially with field at low values of J/t, although this increase is suppressed for higher values of J/t, becoming negligible for $J/t > 0.3$, in a 4×4 cluster with two holes. However, non-negligible field effects are present, up to $J/t = 2.0$, for all distances larger than NN. Above $J/t \approx 0.3$, the field effect at larger distances than NN is quite systematic, as can be seen in figure 6(b) for $J/t = 0.8$, in a 4×4 cluster with two holes ($n_h = 0.125$): the less AF the correlation is, i.e., the larger the distance between the spins, the larger the decrease caused by the field, clearly showing the tendency of the field of trying to decrease the range of the AF SRO. However, it is important to notice that, for this value of J/t, the field effect in the NN correlation is virtually zero. Therefore, for values of J/t where one would expect the AF SRO state to be quite robust, the field does not alter the qualitative aspects of the ground state. This picture remains essentially true down to $J/t \approx 0.3$. Below this value of J/t, there is a qualitative difference in the field effect, since there is a marked *increase* with field in the NN AF correlations. This is clearly seen in figure 6(c), where results at zero (circles) and finite field (triangles) for $J/t = 0.1$ with two holes in a 4×4 cluster clearly show the change from AF to ferromagnetism of the spin correlation at distance $\sqrt{5}$ and the pronounced increase of the NN AF correlation caused by the field. The effect at larger distances can still be described as the field forcing a decrease in the correlation length, but the sharp increase in the NN AF correlation leads us to believe, motivated by the ladder results, that the finite-field ground state is *qualitatively different* from the zero-field ground state. The tentative use of

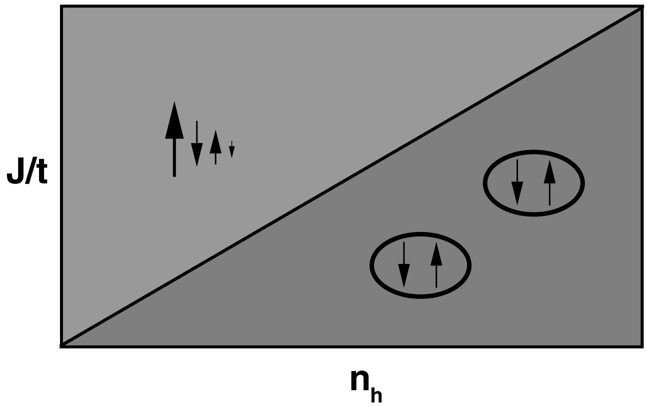

Figure 7. Schematic representation of the phase diagram at finite field. See the text for details. Note that ideally, at the thermodynamic limit, the Nagaoka phase occurs only at $J/t = 0$ and for vanishingly small hole concentration; therefore the phase boundary intercepts the origin.

the term *spin liquid* has its motivation more in the effect of the field in the NN correlations than in the longer range ones. The dependence of the results on hole doping and J/t seems to be consistent with a SL-AF SRO competition. Therefore, this effect could be yet another example of competition between different ground states relevant to the cuprates [40].

A schematic phase diagram at finite field is displayed in figure 7. The main results obtained numerically for the 2D t–J model in the presence of a perpendicular field are presented in a succinct way. In the left region, for high J/t (vertical axis) and small n_h (horizontal axis), the ground state presents AF SRO. Starting from a point inside the left-hand-side region, as one increases J/t and/or decreases n_h (at constant field) the correlation length ξ of the AF SRO increases (the system is drawn away from the phase boundary). On the other hand, if J/t decreases and/or n_h increases, a new ground state with SL characteristics is eventually established (the system crosses the phase boundary to the right-hand-side region). An increase (decrease) of the field will rotate the phase boundary anticlockwise (clockwise), enlarging the SL (AF SRO) phase and squeezing the AF SRO (SL) phase.

It is interesting to note that the effect observed in 4×4 clusters and two-leg ladders is also present in a 2×2 plaquette with one and two holes. As expected, there are qualitative differences: the increase with field in NN AF correlations in a 2×2 plaquette is directly proportional to J/t (therefore it vanishes at $J/t = 0$)[21] and it is an order of magnitude smaller than the increase observed in ladders and 4×4 clusters. Current efforts are under way to try to connect the results in 2×2 to the results described in this paper and possibly gain a qualitative understanding of the magnetic field effect [41].

5. Summary and conclusions

In summary, ED calculations for two-leg ladders and small square clusters have shown that applying a perpendicular magnetic field to the t–J model at low doping tends to induce a SL-like state. In two-leg ladders, the zero-field SL ground state is reinforced by the field,

[21] This is a revealing result. If the change in the correlations from ferromagnetic to AF at $J/t = 0$ in the 4×4 cluster (figure 4(b)) were a finite-size effect, then one would expect it to be preserved as the size of the cluster *decreases*. Although this is not a proof, it suggests that the main effect discussed in this paper is not an artefact of the numerical method.

independently of J/t and doping. Pair breaking caused by the field is clearly observed in ladders and its origin seems to be associated with the decrease with field in the across-the-diagonal AF spin correlation [25]. On the other hand, in 2D this SL state has to compete with the zero-field AF SRO. The spin correlations of the true ground state will then depend on the field strength, the value of J/t and the density of charge carriers. Interestingly, the field effect can be observed in clusters as small as a 2×2 plaquette. As the Hamiltonian in equation (1) can be diagonalized analytically in a 2×2 cluster, a qualitative understanding of the physical origin of the increase of the AF NN correlations may be achieved through a careful analysis of the eigenfunctions. One additional avenue of research worth investigating is how the results presented here will change if hoppings beyond NN are taken in account [26].

Because of the small size of the 4×4 cluster, the authors refrain of making any connection between the results presented here and the experimental results mentioned in the introduction. However, given the relevance of the subject and the lack of calculations including the magnetic field in strongly correlated models like the t–J and Hubbard ones, the authors firmly believe that the results so far presented will stimulate further investigations. In particular, our results predict that an increase in the spin gap of doped ladders with applied field should be experimentally observable.

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