Effects of domain walls on hole motion in the two-dimensional anisotropic $t$-$J$ model at finite temperature

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The $t$-$J$ model on the square lattice, close to the $t$-$J_z$ limit, is studied by quantum Monte Carlo techniques at finite temperature and in the underdoped regime. A variant of the Hoshen-Kopelman algorithm was implemented to identify the antiferromagnetic domains on each Trotter slice. The results show that the model presents at high enough temperature finite antiferromagnetic (AF) domains which collapse at lower temperatures into a single ordered AF state. While there are domains, holes would tend to preferentially move along the domain walls. In this case, there are indications of hole pairing starting at a relatively high temperature. At lower temperatures, when the whole system becomes essentially fully AF ordered, at least in finite clusters, holes would likely tend to move within phase separated regions. The crossover between both states moves down in temperature as doping increases and/or as the off-diagonal exchange increases. The possibility of hole motion along AF domain walls at zero temperature in the fully isotropic $t$-$J$ is discussed.

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The interplay between hole dynamics and magnetic background in the Cu-O plane is considered the central issue in high-Tc superconductivity. This interplay is quite likely essential not only for the mechanism of hole pairing but also for other important features present in the cuprates such as the pseudogap phase and various types of phase separated, inhomogeneous, states.

These problems have been extensively studied by a number of analytical and numerical techniques. One of the most important approaches adopted is through the study of microscopic Hamiltonians, such as the $t$-$J$ model in two dimensions (2D). In particular, numerical techniques have provided a number of highly reliable results for many of the relevant properties which are experimentally measured. Many of these properties are related to the problem of holes and binding of holes in an antiferromagnet. These numerical results were obtained on relatively small clusters as compared, for example, with the antiferromagnetic correlation length in the doped region or with the superconducting coherence length in the superconducting phase. As in these numerical studies (see below), many theoretical scenarios, like the “string” and “spin bag” pictures, assume the presence of an homogeneous antiferromagnetic background.

However, a number of experimental results indicate the presence of various kinds of inhomogeneities, in addition to the most well-known and controversial ones, stripes, which can not easily be included in numerical calculations. Although these inhomogeneities appear in some specific compounds, there is another more universal type of inhomogeneity, in this case of dynamical nature, which are the domain walls (DW) between short range AF regions which appear when doping the AF half-filled insulator. Inelastic neutron scattering studies have shown that the AF correlation length decreases as doping increases. For example, the AF correlation length is between 10 and 20 Å in the doping range $0.04 < x < 0.15$. This finite length of the AF ordered domains is missed in most numerical calculations on small clusters but even in those cases where the largest distance on the cluster studied is about or larger than the AF correlation length, the numerical technique employed should be able to determine these dynamical AF domains and to follow the movement of holes within this array of domains. So far this kind of analysis has not been performed. The closest approach has been done by using density matrix renormalization group (DMRG) techniques. However in this approach, domain walls appear as static features due to the use of open boundary conditions in rectangular clusters.

The effect of domain walls on hole dynamics has been discussed specially in the context of stripes. It has been realized that stripes are essentially DWs with an almost one-dimensional pattern. It is also apparent that holes acquire a larger mobility by moving along these DWs than is discussed.

The purpose of the present study is then to determine the presence of finite AF domains in the 2D $t$-$J$ model and the interrelation between hole movement and do-
main walls. A finite temperature conventional quantum Monte Carlo technique using the checkerboard decomposition is used. This technique allows the study of larger clusters than the ones accessible by exact diagonalization, and more importantly, although working at low hole doping, the number of holes in the system is also much larger. Not only most numerical calculations have so far involved few holes but also analytical approaches, like those mentioned above, are essentially independent particle pictures. On the other hand, it has been noticed that the system with many holes shows a broad range of features, absent in the few holes problem, covered by the concept of “topological ordering”. In fact, not only many holes destroy long range AF order but also the experimental result that spin stripes order at lower temperature is given in units of the concept of “topological ordering”. In standard notation, $t = 1$, $J = 0.35$. Square clusters with side length 8, 10, 12 and 16 with periodic boundary conditions (PBC) and hole doping 0.03 < $x$ < 0.10 are considered. Temperature is given in units of $t$.

It is possible to argue that an enhanced exchange ZZ component appears at an effective level due to interplane exchange coupling. For example, in La$_2$CuO$_{4.11}$ ($x = 0.14$), superconducting below 42 K, there is an AF correlation length in the c-direction that couples a Cu–O$_2$ plane at least with its two (one above, one below) adjacent planes. Although smaller in strength than other 2D interactions (spin-orbit, Dzialoshinskii–Moriya, four-site ring exchange), the inter plane coupling is the responsible for a finite temperature transition at half-filling, below which the correlation length diverges. In any case, we are going to work at very small $\gamma$, i.e. close to the Ising limit of the exchange interaction, or $t$-$J_z$ model, which is not a realistic case for the cuprates but is required to reduce the “minus sign problem” of QMC simulations (see below). In addition, at half-filling, the isotropic 2D Heisenberg model does not have an AF transition at finite temperature (Mermin and Wagner theorem) but the 2D Ising model has a critical temperature of $2.269 J = 0.794 t$. In any case, as far as the interaction between holes and short-range AF order is concerned, the isotropic $t$-$J$ and the $t$-$J_z$ models lead to similar results.

The “minus sign problem” is a very well-known aspect of QMC simulations and it has been extensively analyzed. We give here the outline of the sign calculation in order to make our results fully reproducible. This calculation consists of two parts. First, a local contribution which takes into account fermion permutations inside each cube. Then a global contribution which is due to fermion permutations between different plaquettes at each time slice. The permutations which appear when one hole moves from one side of the cluster to the opposite side have not been included. This is expensive numerically and it is just a boundary contribution. It has been also checked that the influence of this contribution is negligible, at least in the range of temperatures considered. The results shown below have been obtained by averaging at least over six independent runs and at one of the lowest temperatures, $T = 0.3t$, each run consisted of 700,000 MC steps after thermalization. Only the results corresponding to an average sign larger than 0.01 were considered in the present study. The relative error of the measured quantities is around 0.01, i.e. about the size of the symbols used in the plots, except at the lowest temperatures reached, where the error bars are two times larger.

In order to identify the AF domains on each Trotter slice on the square lattice, a variant of the Hoshen-Kopelman algorithm was implemented. This algorithm consists in sweeping each slice row by row. At each site, its state ($z$-projection of the spin) has to be compared with the one of the previous nearest neighbor (NN) site on the same row and with the state of the NN site on the previous row. Two NN sites belong to the same domain if their spins are antiparallel. Care should be taken due to spatial PBC for the last site on each row and for the last row on each slice. Once the domains are identified the number of sites belonging to it is counted. In addition, for all spins belonging to a given domain, the number of neighbors belonging to the same domain and the number of its neighbors belonging to neighboring domains are computed.

We start with a study of the magnetic ordering in the $t$-$J_z$ limit ($\gamma = 0$). In Fig. 1(a) it is shown the dependence with hole doping $x$ of the volume fraction of the two largest domains, $v_1$ and $v_2$ obtained by dividing the number of spins belonging to those domains, $V_1$ and $V_2$, by the number of cluster sites. It can be seen that already at a high temperature, $T \approx t$, there is a large, percolating AF domain occupying roughly half the volume of the lattice. The second largest domain occupies on average roughly one quarter of the lattice, and the relative volume of the third largest domain is smaller than 0.1. One should take into account that for randomly distributed ±1 numbers on a lattice ($T = \infty$ limit), undoped case, the relative volumes are 0.31, 0.17 and 0.10 respectively. As the temperature is lowered, at around $T \approx 0.7t$ (this value decreases as doping increases) there is a rather sharp decrease of the volume of the second largest domain with a consequent increase of the largest domain i.e., the second largest domain collapses into the first one. This change gets smoother as $x$ increases. Below this crossover temperature region, the largest ordered domain occupies 0.95 of the cluster for $x = 0.031$, decreasing smoothly to 0.81 for $x = 0.12$.

In Fig. 1(b) the resulting AF order as seen from $v_1$ and $v_2$ is studied by using a more conventional measure...
of magnetic order, i.e. the spin-spin \((\langle S_i^z S_j^z \rangle)\) correlation function at the maximum distance, \(S_{\text{max}}\). Again there is a steep increase of \(S_{\text{max}}\) as \(T\) decreases presumably indicating a finite temperature transition in the bulk limit. The temperature of this jump decreases from \(T \approx 0.7\), for \(x = 0.039\) (16 \times 16 cluster) to \(T \approx 0.6\), for \(x = 0.097\) (12 \times 12 cluster).

In Fig. 2(a) it is shown the dependence of the volume fraction of the two largest domains \(v_1\) and \(v_2\) with \(\gamma\). Although up to \(\gamma = 0.25\) the results do not depart appreciably from those of the Ising limit, at \(\gamma = 0.5\) it can be observed an important reduction of the volume of the largest domain, and hence in the AF ordering of the system. This behavior of the \(\gamma\) dependence is consistent with the one observed for other quantities as will be shown below, and it suggests that the behavior found for small \(\gamma\) at high temperature is going to remain valid at lower temperatures (and eventually zero temperature) as the isotropic limit is reached. Fig. 2(b) contains a study of the dependence of these domain sizes with cluster size at \(\gamma = 0.5\). The finite size effects are not very important for this anisotropy value and these clusters sizes, although it may become more important as the isotropic Heisenberg case is reached and for smaller sizes. Notice however that there is a slightly larger value of the doping fraction as the linear size is reduced in the data shown in this figure. Hence, if the results were corrected at the same doping fraction, finite size effects would be somewhat larger.

Now, the main point of this study is to detect the location of holes in the presence of ordered AF domains as long as this doped system is approximately described by a \(t-J\) model close to the Ising limit. To get some insight about the microscopic interrelation between holes and AF domains it is useful to look at “snapshots” of the system generated during the QMC simulations. Fig. 3(a) shows a picture at a relatively high temperature \((T = 0.8)\) where there are still ordered domains with the opposite sublattice magnetization (darker shades of gray) than the main ordered domain (lightest shade of gray). The salient feature in this picture is that holes are located preferentially on the boundary of the largest AF domain. There are some other situations that can be identified in this picture, for example isolated holes inside the largest domain with a “string” of overturned spins attached to it.

On the other hand, Fig. 3(b) corresponds to a typical lower temperature behavior. The system presents a single ordered domain occupying most of the cluster and with just few disordered sites. Some features can be identified, such as isolated holes or pairs inside the percolating ordered domain. However, the most important feature is that most holes seems to be located in a phase separated region. In addition, in this and many other snapshots, we observed that most of the spins inside and around this region are ferromagnetically aligned, but we have not studied this issue systematically. Presumably, as AF domains with the opposite magnetization to that of the main one shrink with decreasing temperature, they would leave behind these highly doped regions forming a “mesoscopic” phase separated state or, more properly, a charge inhomogeneous state. In this situation holes would now gain kinetic energy by moving in a ferromagnetic background.

Of course, it is necessary to determine at a more quantitative level the presence of the features shown in Fig. 3. To this end, we adopted the criterion of looking only at the spins and holes belonging to the bulk or to the surface of the largest ordered AF domain, neglecting the

![FIG. 1: Results for the 16 × 16 × γ of magnetic order, i.e. the spin-spin lines and second largest domain (dashed lines). (b) Spin-spin correlations at the maximum distance.](image1)

![FIG. 2: (a) Volume fraction of the largest AF domain (solid lines) and second largest domain (dashed lines), on the 10×10 cluster and various values of the anisotropy γ indicated in the plot. (b) Same as (a) but for γ = 0.5 and various cluster linear sizes and hole densities, indicated in the plot.](image2)
FIG. 3: Snapshot of the 16 × 16 cluster with 16 holes at $T = 0.8$ (top panel) and at $T = 0.4$ (bottom panel). The two lightest shades of gray correspond to spins with the same sublattice magnetization, opposite to that of the two darkest shades of gray. Holes are indicated by circles.

contribution from smaller domains. We believe that this criterion gives the right behavior of the system. Then, for any site belonging to the largest ordered AF domain we computed the number of its nearest and next-nearest neighbor sites belonging to the same domain. We considered a spin in the bulk of the largest AF domain (inner spin) if the number of its neighbors belonging to the same domain is seven or eight, and we consider it at the boundary (boundary spin) if that number is between three and five. We prefer to leave aside the intermediate case of six neighbors and also the case of less than three neighbors, in this case to eliminate some sites which are loosely connected to the main AF domain. In any case, we repeated the calculations taking 2-5 neighbors for the boundary sites and 6-8 neighbors for the inner sites obtaining essentially the same results. We are confident then that the results shown below are quite robust, independent of the details of the classification of spins and holes.

The average fractions of spins located on the boundary ($n^b_i$) and inside ($n^i_i$) the largest AF domain, are defined as the average number of boundary spins divided by the total number of spins in this cluster ($V_1$) and the average number of inner spins divided by $V_1$ respectively. In Fig. 4(a), $n^b_i$ and $n^i_i$ are shown as a function of temperature, at $\gamma = 0$ and other parameters as in Fig. 1. At high temperature the fraction of boundary spins is larger than the fraction of inner ones but this situation is reversed as the temperature is reduced due to the overall ordering of the system. As doping increases, the crossover temperature decreases, consistent with the reduction of AF order with doping. As it can be seen in Fig. 4(b), this crossover temperature is further reduced as the off-diagonal exchange term ($\gamma$) increases. Again, one could expect that the region over which there is an important fraction of boundary spins extends down to zero temperatures at the isotropic limit.

To determine the location of holes with respect to these AF domains, a similar procedure as above was extended to holes. That is, for every hole the number of its nearest and next-nearest neighbor spins belonging to the largest ordered AF domain was computed. As before, we considered a hole located inside the largest AF domain (inner hole) if the number of its neighbors belonging to the same site is seven or eight, and we consider it at the boundary (boundary hole) if that number is between three and five. The average fraction of boundary holes ($n^b_h$) and the average fraction of inner holes ($n^i_h$) are obtained by dividing the number of boundary holes and the number of inner holes respectively, by the total number of holes.

Results of these calculation are depicted in Fig. 5. The overall features are similar to those of Fig. 4, i.e. there is a dominance of boundary holes at higher temperatures changing to inner holes at lower temperatures (Fig. 5a)). The fact that this crossover temperature at a given doping is lower than the corresponding temperature for spins suggests that holes have a preference to be located at the boundary, a possibility that will be confirmed below. Fig. 5b) also shows that this crossover temperature is
FIG. 5: Average fraction of holes located on the boundary (dashed lines) and inside (solid lines) the largest AF domain as a function of temperature. (a) Same clusters and hole filling as in Fig. 4, \( \gamma = 0 \). (b) Same clusters and parameters as in Fig. 4(b).

Reduced by increasing \( \gamma \) again consistent with the results of Fig. 4(b). Another feature that can be observed is that at the lowest temperatures, the reverse behavior occurs, i.e., there is an increase (decrease) of the boundary (inner) hole fractions. It is easy to see that this behavior is consistent with the formation of a phase separated hole-rich region inside the main AF percolating domain. This possibility is also examined below.

The central problem of the interrelation between holes and AF domains is addressed in Fig. 6, where the ratio \( r_b^h \) of the fraction of boundary holes to the fraction of boundary spins is shown. This quantity, obtained from two quantities computed in QMC simulations, have then larger error bars than the ones of those quantities. The main result is that the ratio \( r_b^h \) is always noticeably larger than one indicating a preference of the holes to move along the boundary of AF domains. In Fig. 6(a), it is shown that \( r_b^h \) increases as \( T \) is reduced, and decreases as doping increases. In Fig. 6(b), it is also shown that \( r_b^h \) decreases as \( \gamma \) increases. It is out of question to perform an extrapolation to \( \gamma = 1 \) but this behavior suggests that one should be cautious about extending the conclusions of the present study to the isotropic case. The inset of Fig. 6(b) shows the hole population of the domain walls, \( p_w \), defined as the number of holes on the boundary of the largest ordered domain divided by the number of spins (i.e., the “length”) of this boundary. It turns out that \( p_w \) is just \( r_b^h \) multiplied by the hole density \( x \) and divided by \( v_1 \). To take a reference, on the stripes \( p_w = 0.5 \), which seems considerably higher than an extrapolation to zero temperature of the present data, specially taking into account the reduction with increasing \( \gamma \).

An elementary argument of minimization of the number of broken AF bonds leads to the possibility of pairing of holes even when they are constrained to move along the boundary between AF domains. In order to confirm this possibility, and to get further indications of the presence of a low temperature phase separation, we computed the hole-hole correlations \( C(r) \) as a function of temperature. In Fig. 7(a) these correlations are shown as a function of distance and at various temperatures for a fixed value of \( x \) and \( \gamma \). As \( T \) decreases, the correlations at large distances decrease while the correlations at short distances increase indicating the onset of hole attraction. Quite interesting, at intermediate temperatures, the largest correlation corresponds to the distance of \( \sqrt{2} \), as was observed in many numerical studies for two holes at zero temperature in the fully isotropic \( t-J \) model and this is typical of \( d_{x^2-y^2} \) pairing. At the lowest temperature, the correlations are enhanced both at near and at far distances and suppressed at intermediate distances which is typical of a phase separated state.

For better visualizing the attraction between holes we averaged \( C(r) \) for \( r = 1, \sqrt{2} \) and compared it with the average over the three largest distances on the cluster. Fig. 7(b) shows these averages as a function of temperature, on the \( 12 \times 12 \) cluster, \( \gamma = 0 \) and at various dopings. It can be seen that the crossover temperature at which the near distance correlations start to dominate over the long distance ones, i.e. the probability of finding two holes becomes larger at short distance than at long distance, decreases slightly as a function of doping (of course, error bars exclude a precise determination of this crossover). This crossover temperature could be identified with \( T^{MF} \) as discussed in Ref. 24. Fig. 7(c) seems also to indicate that the pairing crossover temperature, for a given cluster size and doping, decreases with
increasing $\gamma$. One should stress the fact that this onset of pairing takes place while there is still a larger fraction of holes on the DW than inside the largest ordered AF domain. For example, from Fig. 7(b), the onset of pairing occurs approximately at $T = 0.76$, 0.70 and 0.66, at $x = 0.056$, 0.069 and 0.083, respectively. The corresponding crossover from DW hole fraction to bulk hole fraction (Fig. 7(a)) takes place at $T = 0.69$, 0.66 and 0.60 for the same fillings.

It is also worth to mention that by looking at hole-hole correlations in momentum space we have not found indications of stripe formation. This hole static structure factor is loosely distributed around $(0,0)$ with not definite pattern. Presumably, additional mechanisms have to be invoked to stabilize a stripe state. The peak of the magnetic structure factor is also always at $(\pi, \pi)$. In addition, by examining snapshots like the ones in Fig. 7 and by computing a measure of compactness using the data of Fig. 4, it turns out that the AF domains are in close contact between each other and are far from being "round" objects as implicitly assumed in Ref. 2. Hence, also in this type of inhomogeneity an external agent should be present to stabilize the reported static AF islands.

Let us summarize and discuss the main results of the present study. The 2D exchange anisotropic $t$-$J$ model, close to the $t$-$J_z$ limit, presents at high enough temperature finite AF domains which, at least in finite clusters, collapse at lower temperatures into a single ordered AF state. While there are domains, and hence domain walls, holes would tend to preferentially locate along these DW. In this case, there are indications of hole pairing starting at a relatively high temperature. One could speculate that this situation extends down to zero temperature in the fully isotropic $t$-$J$ model as this model is supposed to describe, for the appropriate hole doping, the superconducting phase of the cuprates. On the other hand, the fully isotropic case may behave as the $t$-$J_z$ model behaves at zero temperature, at least in finite clusters, and in this case it could undergo a crossover to a charge inhomogeneous state. As mentioned in the introductory paragraphs, there are many experimental indications of various kinds of inhomogeneities in the cuprates. In any case, the nature of the possible charge inhomogeneous state detected in the simulations should be further analyzed.

A possible consequence of the reduction of the boundary length as temperature is decreased, is that the holes would become increasingly localized. This localization could contribute to the increase of in-plane resistivity in lightly doped $La_{2-x}Sr_xCuO_4$ and $YBa_2CuO_4$ as $T$ is reduced reported in recent experimental studies. An indirect support to this scenario comes from the relation between resistivity and AF correlation length in $La_{2-x}Sr_xCuO_4$. It can be seen (Fig. 3 of Ref. 25) that the inverse mobility and the AF correlation length $\rho_{AF}$ have an identical behavior as a function of doping. However, one should be cautious since the mobility is measured at room temperature while $\rho_{AF}$ is the zero temperature value. Of course, in these compounds, stripes, which are a particular kind of DW, could be stabilized. In addition, the kinetic energy, computed in our simulations, is almost constant down to the lowest temperatures attainable. Perhaps, the system responds to this tendency to localization by going into a charge inhomogeneous state. In any case, one could suggest recipes to avoid this tendency to localization due to the shrinking of AF domains, present in all cuprates. For example, DWs could be enforced into the system by introducing magnetic impurities outside CuO$_2$ layers in order to pin domains with random sublattice magnetizations. The resulting enlarged DW length would reduce hole localization and prevent phase separation.

Finally, let us compare the present results with the ones obtained in some of the most recent and closest studies. In the first place, in Ref. 15, DWs are essentially straight lines, and essentially static, both in their analytical treatment and in their DMRG calculations. Hence their predictions are of limited applicability in the finite temperature real physics of the $t$-$J_z$ model, as revealed by the present simulations, where dynamical domains are considerably non-compact regions. In particular, our main result, holes moving essentially along DWs, suggests that “transverse” motion of holes is unlikely. Notice also that, by looking at the present results on a larger “time scale”, the AF domains could appear as more compact regions separated by broadened disordered domain walls. In addition, Ref. 16 is a study at zero temperature, where we obtain, with PBC, indications of clustering of holes. In this sense, their zero temperature DW should be a consequence of additional effects not in-
cluded in the \( t-J_z \) model. In our case, finite AF domains appear as a competition between charge and magnetic energy, at finite temperatures. The issue of domain wall formation in our model has to be further investigated and it would be useful to compare the wall energetics with the predictions of Ref. 13. Another of our most important results are the indications of binding of holes. This is a delicate issue which has been hotly debated in the context of stripes. 14,15 In Ref. 15 it was concluded that the presence of a DW is mostly irrelevant to pairing. In studies where charge stripes are forced into the system by an on-site potential added to an anisotropic \( t-J \) model, no indications of pairing were found: stripes are metallic. In these studies, spin and hole correlations along the stripe are very much similar to the ones in isolated \( t-J \) chains.

One may suggest then, that the behavior of dynamical domain walls studied in the present work is considerable different than for stripes where charge is ordered by an external mechanism.

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