An exact diagonalization demonstration of incommensurability
and rigid band filling for N holes in the $t-J$ model

R.J. Gooding, K.J.E. Vos

Dept. of Physics, Queen’s University,
Kingston, Ontario K7L 3N6

P.W. Leung

Dept. of Physics, Hong Kong University of Science and Technology,
Clear Water Bay, Hong Kong

(September 16, 2018)
Abstract

We have calculated $S(\vec{q})$ and the single particle distribution function $< n_{\vec{q}} >$ for $N$ holes in the $t - J$ model on a non-square $\sqrt{8} \times \sqrt{32}$ 16–site lattice with periodic boundary conditions. We justify the use of this lattice by appealing to results obtained from the conventional $4 \times 4$ 16–site cluster, and an undoped 32–site system, each having the full square symmetry of the bulk. This new cluster has a high density of $\vec{k}$ points along the diagonal of reciprocal space, viz. along $\vec{k} = k(1, 1)$. The results clearly demonstrate that when the single hole problem has a ground state with a system momentum of $\vec{k} = (\frac{\pi}{2}, \frac{\pi}{2})$, the resulting ground state for $N$ holes involves a shift of the peak of the system’s structure factor away from the antiferromagnetic state $\vec{q} = (\pi, \pi)$. This shift effectively increases continuously with $N$. When the single hole problem has a ground state with a momentum that is not equal to $\vec{k} = (\frac{\pi}{2}, \frac{\pi}{2})$, something that may easily be accomplished through the use of the $t - t' - J$ model with $t'/t$ small and positive, then the above–mentioned incommensurability for $N$ holes is not found – the maximum of $S(\vec{q})$ remains at $\vec{q} = (\pi, \pi)$ for all $N$. The results for the incommensurate ground states can be understood in terms of rigid–band filling: the effective occupation of the single hole $\vec{k} = (\pm\frac{\pi}{2}, \pm\frac{\pi}{2})$ states is demonstrated by the evaluation of the single particle momentum distribution function $< n_{\vec{q}} >$. Unlike previous studies, we show that for the many hole ground state the occupied momentum states are indeed $\vec{k} = (\pm\frac{\pi}{2}, \pm\frac{\pi}{2})$ states. These conclusions are in agreement with the predictions for the spiral phase made by Shraiman and Siggia. Further, our results demonstrate that in some instances important results of moderately doped $CuO_2$ planes can be predicted from a knowledge of the properties of weakly doped planes.
I. INTRODUCTION:

The $CuO_2$ plane based high–temperature superconductors have anomalous normal state properties, and it is probable that a complete theory of the superconducting instability will first require a theory of this phase. One part of the normal state puzzle involves the spin dynamics, and in $La_{2-x}Sr_xCuO_4$ for $x = 0.075$, 0.14 and $x = 0.15$ recent experiments [1–3] have demonstrated the existence of incommensurate magnetic fluctuations. An explanation of these results is an outstanding theoretical problem.

One theoretical starting point for these materials is the strong coupling limit of the Hubbard model [4], and it has been argued that the simpler $t – J$ model [5] adequately represents the important low–energy physics of these systems. Then, the question is: do the predictions of the normal state properties extracted from the $t – J$ model agree with experiment? Here we shall focus on the predictions of the magnetic features of these systems that can be made from the strong–coupling limit. Numerous theoretical treatments [6–11] of this problem have indeed suggested that some form of a magnetic instability towards an incommensurate phase may arise in this model. Unfortunately, not all of these theories agree with one another, so more work is required to clarify the situation.

As elaborated in a review by Dagotto [12], one avenue by which theorists may scrutinize theoretical predictions involves the use of exact diagonalization techniques. This allows for the complete determination of all eigenstates of a given system. The limitation of this method is simply the rather small systems that can be studied, and thus comparisons of theory to experiments on bulk systems can be quite limited. Progress is being made, and recent sophisticated techniques have been developed to treat somewhat larger Hilbert spaces. One finite–size scaling study [13] of a doped $t – J$ model yielded the encouraging result that the commonly used $4 \times 4$ 16–site square lattice has only small finite size effects, at least for one hole.

An exact diagonalization study of the $t – J$ model for a variety of carrier densities was performed by Moreo et al. [14]. These studies were conducted before the above–mentioned
experiments [1–3], and thus Moreo et al. focussed on a search for an incommensurate phase that was stable in the thermodynamic limit. We now know that the incommensurability is only found in the spin dynamics, and thus different questions are important. To be specific: (i) what kind of incommensurability (if any) is actually found in the $t – J$ model, and (ii) what are the underlying states that the carriers occupy when in such a state?

To make clear the relevance of the latter question, consider that using the $t – J$ model Shraiman and Siggia [6] have predicted the development of an incommensurate spiral phase as a CuO$_2$ plane is doped away from half filling. Implicit in the development of their theory of the spiral phase is the assumption that at very low doping levels the carriers approximately exist in momentum states corresponding to the ground state of the one–hole problem. (The one–hole problem has been studied using a variety of techniques, and it is well known [15–17] that the ground state has a system momentum $\vec{k} = (\pm \pi 2, \pm \pi 2)$. This has been confirmed by various exact diagonalization studies [12], including the finite–size scaling work [13] mentioned above.) Thus, the resilience of some form of rigid band filling around so–called hole pockets is crucial if the instability suggested by Shraiman and Siggia is to be validated. Since recent photoemission work [18] on YBa$_2$Cu$_3$O$_{6.35}$ have found partial evidence for the hole pocket picture in the low doping regime, this question is clearly very important.

The potential success of Ref. 6 in predicting the magnetic features of the moderately doped high $T_c$ superconductors is related to an even bigger and more important question: can lessons learned from studying the properties of the weakly doped CuO$_2$ planes, e.g. the single hole problem, be used to correctly extrapolate to higher doping levels? We now know that at least for small but nonzero doping levels this may be the case: For one hole localized by a divalent Sr impurity, theory has predicted the ground state [19–21]. The magnetic component of the ground state was identified [21], and based on the above–mentioned semi–classical field theory of Shraiman and Siggia [16] it was realized that a two–fold degenerate non–coplanar spin texture was present. (This spin state may be thought of as that resulting from a particular superposition of ferromagnetic bonds [22] in a 2D antiferromagnetic lat-
tice [21].) Then, experiment showed [23] that such a model [24,25] correctly reproduced the zero–temperature antiferromagnetic correlation length. More recently it was demonstrated that this is also true for nonzero temperatures [25]. Lastly, using La NQR [26] it has recently been observed that at very low dopings and low temperatures, coexisting with long–ranged antiferromagnetic order is a transverse spin freezing - the temperature at which the freezing occurs may be analytically predicted [27] using either the semiclassical field theory, or accurately predicted numerically [27] using the model employed in Ref. 25. These successes suggest that perhaps one might be able to continue to extrapolate the semiclassical theory to even higher doping levels, and this possibility, along with the experiments [1] consistent with the spiral phase [6], were the initial motivation for this paper.

Thus, here we will present two correlation functions measured using ground states obtained from an exact diagonalization study of the $t – J$ model for metallic densities of carriers. We focus on the two questions mentioned above, viz. (i) is there any evidence that at non–zero doping levels the ground state for the $t – J$ model displays any hints of incommensurability, and (ii) if so, which single–particle states are occupied in the incommensurate phase. Our results will provide some justification for the spiral phase arguments made by Shraiman and Siggia, as well as for the similarities of the ground states for the weak and moderate doping regimes. Our paper is organized as follows. In §II we introduce the cluster on which the exact diagonalization determination of the ground state was accomplished. We justify the use of this non–standard, non–square lattice by appealing to exact diagonalization results obtained on other lattices possessing the full square symmetry of the plane. In §III we describe the magnetic properties of N holes subject to the $t – J$ model for this cluster; we focus on the static structure factor, $S(q)$, and show that as the cluster is doped, the peak in $S(q)$ shifts away from the antiferromagnetic wave vector. Then, in §IV we consider the $t – t’ – J$ model, and demonstrate what happens when the single hole ground state has a crystal momentum that is not at $k = (\pm \pi, \pm \pi)$: simply, the above mentioned incommensurability is no longer found. In §V we analyse the occupation of the single particle momentum states – we show that for the one, two, three, and four hole systems,
the occupation of the associated momentum states is not unlike the situation that would be predicted via rigid band filling arguments. Finally, in §VI we discuss our numerical results, focusing on comparisons to other theories and previous exact diagonalization studies.

II. DESCRIPTION AND PROPERTIES OF NON–SQUARE 16–SITE CLUSTER:

Exact diagonalization is now a familiar technique by which studies of systems with small Hilbert spaces can be carried out. For two-dimensional, $S = \frac{1}{2}$ quantum spin systems (including doped quantum antiferromagnets, a strong-coupling model of the high-temperature superconductors) the most commonly studied Hilbert space corresponds to a square $4 \times 4$ cluster with periodic boundary conditions. Since a cluster of spins is supposed to represent a portion of the bulk of the crystal, it has always been thought to be desirable to ensure that the symmetry of the bulk be maintained in the cluster. In this section we will introduce a non–square cluster of 16 spins with periodic boundary conditions. Then, we will justify the use of this lattice by comparing to results for clusters which have the full square symmetry, and, in fact, we will see that some of the unphysical results obtained with the square 16–site cluster are eliminated when our non–square cluster is used.

Figure 1 shows a cluster of sites which represent a small portion of a bulk, two-dimensional square lattice; in total, it contains 32 sites. Also, this cluster has the full $4mm$ point group symmetry of the bulk lattice (though obviously not the translational periodicity of the infinite square lattice). We impose periodic boundary conditions on this cluster, and this yields the reciprocal lattice vectors shown in Fig. 2a.

Our non–square 16–site lattice is also shown in Fig. 1 – it is outlined by the rectangle elongated along the (1,1) direction, and may be referred to as a $\sqrt{8} \times \sqrt{32}$ lattice. Clearly, it has a lower point group symmetry, viz. it only possesses a centre of inversion symmetry. Imposing periodic boundary conditions, the reciprocal lattice vectors for this cluster are shown in Fig. 2b – note that due to the lack of square symmetry of this cluster $\vec{k} = (k_x, k_y)$ is not necessarily equivalent to $(k_y, k_x)$. 
Our motivation for choosing this cluster is two fold. Firstly, we wish to dope this lattice and determine whether or not there is any sign of incommensurability in the many–hole ground state. If the ordering wave vector shifts continuously (with doping) away from the ordering wave vector for the commensurate antiferromagnetic insulator state, \( \vec{q} = (\pi, \pi) \), then we should employ a cluster that has as many reciprocal lattice vectors close to \((\pi, \pi)\) as possible. As seen in Fig. 2b, our non–square 16–site lattice has a multitude of \( k \) points along the zone diagonal that are close to \((\pi, \pi)\), viz. \( \vec{k} = (\pi, \pi), \left(\frac{3\pi}{4}, \frac{3\pi}{4}\right), \left(\frac{\pi}{2}, \frac{\pi}{2}\right) \), and \( \vec{k} = \left(\frac{\pi}{4}, \frac{\pi}{4}\right) \). Secondly, if any incommensurability is found in our studies, we wish to understand the origin of the possible instability that leads to the incommensurate state. Thus, if we are going to scrutinize the above mentioned theories, we should not eliminate the proposed progenitors of the incommensurability. Here we shall focus on whether or not the holes tend to form many-hole wave functions that are essentially constructed from a rigid band filling of the associated one–hole ground states. The important (low energy) one hole states are \( \vec{k} = (\pi, 0) \), and \( \vec{k} = \left(\frac{\pi}{2}, \frac{\pi}{2}\right) \), and as shown in Fig. 2b, our non-square 16–site cluster does indeed possess both of these reciprocal lattice vectors. Thus, the 16–site non–square cluster shown in Fig. 1 is ideal for our purposes if its lack of square symmetry does not produce any anomalous results; we now show that this is indeed the case.

**A. Behaviour of the Undoped Non–Square 16–Site Cluster:**

We have evaluated the ground state, and first excited state, for the 32 and 16–site clusters shown in Fig. 1, as well as for the common \( 4 \times 4 \) square cluster, for the antiferromagnetic Hamiltonian

\[
H = J \sum_{<ij>} \vec{S}_i \cdot \vec{S}_j \tag{2.1}
\]

when an \( S = \frac{1}{2} \) spin is placed at every site of the cluster, and periodic boundary conditions are used. For all three clusters the ground state was a \( \vec{k} = 0 \) singlet; for the two 16–site clusters, the ground state energies per spin were found to be very close to one another:
-.7018 for the $4 \times 4$ cluster, and -.7085 for the non–standard 16–site cluster. Further, the first excited state for all three clusters was always found to be a $\vec{k} = (\pi, \pi)$ triplet; for the two 16–site clusters the mass gap (per site) was found to be very close: .0723 for the $4 \times 4$ cluster, and .0740 for the non–square cluster.

We are interested in the magnetic structure factor of the doped lattice; thus, we must be sure that the non–square 16–site cluster does not yield any anomalous results for this quantity. The magnetic structure factor corresponds to

$$S(\vec{q}) = \frac{1}{N} < GS^n_{\vec{k}} | \left[ \sum_{i,j} e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)} \vec{S}_i \cdot \vec{S}_j \right] | GS^n_{\vec{k}} >$$

where $| GS^n_{\vec{k}} >$ is the ground state for $n$ holes having system momentum $\vec{k}$, and $N$ is the total number of sites. In Fig. 3 we show this quantity for all three clusters; since the reciprocal lattice points do not always overlap, the comparison can only be made at certain points. It is clear that all three clusters give the same general features. Further, and most importantly to this study, for the $\vec{q}$ along the zone diagonal, the 32–site cluster and our non-square 16–site cluster have very similar static structure factors. For example, for $\vec{q} = (\frac{\pi}{2}, \frac{\pi}{2})$ all three clusters have near identical values of $S(\vec{q})$.

It is apparent from these results that no anomalous features arise when the non–square cluster is used for an undoped Heisenberg Hamiltonian; we now consider the doped cluster.

**B. Behaviour of the Doped Non–Square 16–Site Cluster:**

We have investigated the $t – J$ model, defined by

$$H = -t \sum_{<i,j> \sigma} (\tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} + h.c.) + J \sum_{<ij>} (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j)$$

where we choose $t = 1$ and $J = .4$, as representative of a $CuO_2$ plane. The operators $\tilde{c}_{i\sigma}^\dagger, \tilde{c}_{i\sigma}$ are the creation and annihilation operators, respectively, corresponding to the Hilbert space which has been reduced by having had all doubly occupied sites integrated out; the notation $<i,j>$ implies that only near–neighbour pairs are summed over.
We added a single hole to the half–filled, antiferromagnetic insulator; then, the minimum energy state was determined for every allowed system momentum for both sixteen site clusters. The results, cast in the form of a “band” structure, are shown in Fig. 4. The variation of energy with respect to wave vector is seen to be similar for the two clusters, although the band width for the non–square cluster is smaller than for the square cluster.

One intriguing advantage to the use of the non–square cluster is quickly recognized from these results. To be specific, for one hole and the \( t – J \) Hamiltonian, use of the \( 4 \times 4 \) square cluster yields the entirely unphysical result that all states with system momenta \( \vec{k} = (\pi, 0) \) and \( (\frac{\pi}{2}, \frac{\pi}{2}) \) (and, of course, those \( \vec{k} \) points related to these by the \( 4mm \) square symmetry) are degenerate; a proof of this fact may be found elsewhere [28]. This is unfortunate since these two states will be non–degenerate in the bulk limit. Further, theory predicts that these two states are the two lowest energy states assumed by a single hole. Our non–square 16–site cluster is very useful in that it contains all of these \( \vec{k} \) points, and also has a sufficiently small Hilbert space such that the one hole states can be accessed, but there is no artificial (geometry–imposed) degeneracy between \( \vec{k} = (\pi, 0) \) and \( \vec{k} = (\frac{\pi}{2}, \frac{\pi}{2}) \). From Fig. 4 it is seen that the single hole ground state for the non–square cluster is \( \vec{k} = (\frac{\pi}{2}, \frac{\pi}{2}) \), and \( (\pi, 0) \) is an excited state; this is consistent with the conclusions that have been reached regarding the single hole problem [15,16]. (One persistent disadvantage found when using this cluster for one hole is that for \( k_x – k_y = \pm \pi \), the minimum energy states are degenerate; the same phenomenon occurs for the square 16–site cluster. Only the degeneracy along \( k_x + k_y = \pm \pi \) found in the square 16–site cluster is removed when we use the non–square cluster.)

Summarizing this section, we have introduced a non–square 16–site cluster with periodic boundary conditions. Important reciprocal lattice points are present in this lattice, and in comparison to the square \( 4 \times 4 \) 16–site cluster certain artificial degeneracies are lifted. No anomalous results were found for the undoped or singly doped non–square cluster.
III. INCOMMENSURABILITY VS. NUMBER OF HOLES:

We have used exact diagonalization to find the ground state of the $t - J$ Hamiltonian for the non-square 16-site cluster for one through four holes [29]; this corresponds to doping levels of $x = 0.0625$ to $x = 0.25$, and covers the experimental range of interest for systems that have displayed incommensurability [1–3].

The ground states, for $t = 1$ and $J = 0.4$, for $N = 1$ and 2 holes have crystal momenta $\vec{k} = \pm\left(\frac{\pi}{2}, \frac{\pi}{2}\right)$, and $\pm(\pi, \pm\pi)$, respectively. For 3 holes the ground state is highly degenerate at the following reciprocal lattice points: $\pm(-\pi, 0), \pm(-\frac{3\pi}{4}, \frac{\pi}{4}), \pm(-\frac{3\pi}{4}, \frac{3\pi}{4}), \pm(-\frac{\pi}{4}, \frac{3\pi}{4})$, and $\pm(0, \pi)$. For 4 holes the ground state is found to correspond to momenta $\pm\left(\frac{\pi}{2}, \frac{\pi}{2}\right)$.

We have calculated the static structure factor, defined in Eq. (2.2), and our results are shown in Fig. 5. The maximum of $S(\vec{q})$ occurs at a wave vector which shifts from $(\pi, \pi)$ (the antiferromagnetic wave vector) for one and two holes, to $(\frac{3\pi}{4}, \frac{3\pi}{4})$ for three holes, to $(\frac{\pi}{2}, \frac{\pi}{2})$ for four holes. (Note that for ground states with non-zero crystal momenta, one should perform an average over the set of ground state wave functions that are degenerate (due to the degeneracy of the ground state with respect to differing $\vec{k}$ points); here, for 1, 2, and 4 holes, due to the lack of mirror symmetry about the $x$ and $y$ axes for our non-square cluster, this does not change the results that are obtained when performing this average, viz. only $\vec{k}$ and $-\vec{k}$ are degenerate, and $S(\vec{q})$ is insensitive to which of these ground state eigenfunctions is used. For 3 holes the same structure factor is obtained for all of the degenerate wave vectors.)

As the second hole is added, all that happens is a reduction of the antiferromagnetic correlations - this may also be seen in another correlation function, viz. the relative decrease of the near-neighbour spin-spin correlation function $\langle \vec{S}_i \cdot \vec{S}_j \rangle$. Then, for three and four holes, an essentially continuous shift in peak position occurs; the continuous shift in wave vector is seen to mimic the experiments of Cheong et al. [4]. For more than four holes, $S(\vec{q})$ is essentially flat, indicating the effective loss of magnetic correlations in the heavily doped materials.
It would be desirable to be able to perform the same search for incommensurability on a lattice with a high density of $\vec{k}$ points around $(\pi, \pi)$ such that the neighbouring $\vec{k}$ points were along the $(1,0)$ and/or $(0,1)$ direction; this is the direction of the incommensurate shifts found experimentally [1]. However, the only lattice (with a small number of sites, and thus appropriate for exact diagonalization studies of a multiply doped cluster) is that of a ladder of width two - this cluster would in no way approximate the bulk lattice, and thus we must be content with a search for incommensurabilities along the zone diagonal. Further, it has been suggested, in a weak coupling theory, that one cannot reproduce the experimentally observed shifts in a one–band model; instead, a three-band model is required to produce the necessary nesting [30]. Even if we had used a three–band model, the nature of our cluster still restricts us to the set of $\vec{k}$ points explored here, and thus we do not believe studies of $S(\vec{q})$ on finite clusters in the strong coupling limit could yield more information on the incommensurability than we have found until the technical obstacles associated with doping a 32, or 36–site cluster [13,31] with many holes are overcome - this may never be possible. Further, only with such progress could the finite–size scaling be carried out to scrutinize the observation [2] that a very weak logarithmic maximum of $S(\vec{q})$ exists at the incommensurate wave vectors.

IV. INCOMMENSURABILITY IN THE $t–t’–J$ MODEL:

We have considered the ground state of the $t–t’–J$ model. This model corresponds to the Hamiltonian of Eq. (2.3) augmented with a next nearest neighbour hopping:

$$H' = -t' \sum_{<i,i'>\sigma} \left( \hat{c}^\dagger_{i\sigma} \hat{c}_{i'\sigma} + h.c. \right)$$

(4.1)

where $i'$ is a next near neighbour to $i$. The inclusion of this new term has been motivated in a variety of ways [32–34]; here it is extremely useful in showing how the incommensurability demonstrated in the above section is changed when the crystal momentum associated with the single hole problem is shifted away from $\vec{k} = \pm(\pi/2, \pi/2)$. For $t = 1$. and $J = .4$, we have
added a small positive $t'$, viz. $t' = .2$, and found the ground state for our non–square 16–site cluster. The ground state momentum is no longer at $\vec{k} = \pm(\frac{\pi}{2}, \frac{\pi}{2})$, but now is found to be at $\vec{k} = \pm(\pi, 0)$. This behaviour is consistent with the band–structure predictions for a hole moving in an inert background.

In Fig. 6 we show $S(\vec{q})$ for 1, 2, 3, and 4 holes, for the $t - t' - J$ model, using the model parameters given above. It is clearly seen that the maximum of the magnetic structure factor is always at the antiferromagnetic wave vector, viz. $\vec{q} = (\pi, \pi)$. As the cluster is progressively doped, all that happens is a suppression of the antiferromagnetic correlations - no shift of $S(\vec{q})$ to wave vectors neighbouring the antiferromagnetic $(\pi, \pi)$ is found. (As mentioned above, this is also found when studying the near–neighbour spin–spin correlation function $<\vec{S}_i \cdot \vec{S}_j>$. ) This is in marked contrast to the behaviour found in the above section: cf. Fig. 5. This simple demonstration seems to suggest that in the strong–coupling limit the formation of an incommensurate phase requires the single hole problem to have its ground state momentum equal to $\vec{k} = (\frac{\pi}{2}, \frac{\pi}{2})$. We now examine the single particle momentum distribution function to show why this is so.

V. MOMENTUM DISTRIBUTION FUNCTIONS:

In the previous two sections we have displayed results obtained from exact diagonalization studies that provide evidence for incommensurate correlations in the strong coupling limit of a two–dimensional doped antiferromagnetic insulator when the single hole ground state was located at $\vec{k} = \pm(\frac{\pi}{2}, \frac{\pi}{2})$. The question that naturally arises is: why does the one hole state so profoundly affect the many hole features? In this section we wish to show that one can also use the exact diagonalization results to suggest the progenitor of this incommensurability, and subsequently answer this question via a study of the electron and hole momentum distribution functions.

Our approach is very similar to one employed by Stephan and Horsch [35], as well as that more recently given in a very clear presentation made by Ding [36] - in our work we...
shall follow the notation of Ding. One defines the electron distribution function by

\[ < n_\sigma(\vec{q}) >= < \tilde{c}_\vec{q}^{\dagger} \tilde{c}_{\vec{q}\sigma} >. \] (5.1)

Similarly, a hole momentum distribution function can be defined:

\[ < p_\sigma(\vec{q}) >= < \tilde{c}_\vec{q} \tilde{c}_{\vec{q}\sigma}^{\dagger} >. \] (5.2)

Note that in using this definition, the hole distribution function includes a spin index, a feature induced by the constraint of no double occupancy - this property is explained by Ding [36]. We wish to track the electron and hole occupations as our cluster is doped from one to four holes. To be specific, we wish to ascertain which electron and hole states are occupied as the incommensurability found in the previous section develops.

If one examines these distribution functions for the \( t' = 0 \) ground states discussed above, one must overcome more unphysical degeneracies; e.g., the four hole \( < n_\sigma(\vec{q}) > \) has degenerate values for \( q_x - q_y = \pm \pi \). Further, the analysis is greatly complicated by the degeneracy (with respect to the wave vector) of the many-hole ground states; e.g., the unphysical degeneracy of the 3 hole state. This problem for the non-square 16-site cluster is unique to the pure \( t - J \) model. To remove it one can add the second near-neighbour hopping \( t' \) introduced in §IV - it is known that this hopping amplitude is of opposite sign to that of the near neighbour hopping [32]. We have chosen \( t'/t = - .1 \) for a number of reasons: (i) with this addition the degeneracies of the many hole ground states are lifted, (ii) the single hole ground state remains at \( \vec{k} = \pm (\frac{\pi}{2}, \frac{\pi}{2}) \), and in comparison to the \( t' = 0 \) system, the ordering of the low energy excited states is not changed, and (iii) the two and four hole ground states become \( \vec{k} = 0 \) states, a property that one certainly would expect a bulk system with an even number of holes to possess. As an example of the usefulness of including the second near neighbour hopping, note that when \( t' = 0 \), the three hole ground state on our non-square 16-site cluster is degenerate at the following wave vectors:

\[ \pm(-\pi, 0), \pm(-\frac{3\pi}{4}, \frac{\pi}{4}), \pm(-\frac{\pi}{2}, \frac{\pi}{2}), \pm(-\frac{\pi}{4}, \frac{3\pi}{4}), \pm(0, \pi). \] Then, when \( t' = - .1 \) is added, one finds that this unphysical degeneracy is lifted and the ground state occurs at \( \pm(\frac{\pi}{2}, -\frac{\pi}{2}) \). We wish
to stress that identical conclusions to the ones presented below can be reached for any small and negative $t'$ \[37\].

For 1, 2, 3, and 4 holes in the $t-t'-J$ model with $t = 1$, $J = .4$, and $t' = -.1$, on our non-square 16–site cluster the ground state is found to occur at $\vec{k} = \pm(\frac{\pi}{2}, \frac{\pi}{2})$, $(0, 0)$, $\pm(\frac{\pi}{2}, -\frac{\pi}{2})$, and $(0, 0)$, respectively. Then, the electron and momentum distribution functions are as shown in Figs. 7, 8, 9, and 10. For an odd number of holes we show both spin components of the distribution functions; for an even number we show just one of the two spin components for both the electrons and holes (since the up and down spin distributions are equivalent). Various sum rules, etc., associated with these numbers are discussed at length by Ding \[36\]. The positioning of these numbers in the figures corresponds to the allowed wave vectors of the non–square 16–site cluster, as shown in Fig. 2b.

The one hole ground state (which was found in the subspace of the total magnetization being $\frac{1}{2}\hat{z}$) clearly shows the large occupation of the electron states within the antiferromagnetic Brillouin zone (defined by $|q_x| + |q_y| = \pi$) except for electrons and holes at the wave vector of the ground state, i.e. $\vec{k} = \pm(\frac{\pi}{2}, \frac{\pi}{2})$; only one of these electron states is found to be occupied. This is the same result as was found by Ding \[36\], and shows that one may associate the momentum of the ground state, and the momentum of the hole state, to be one and the same for one hole even in the strong coupling limit. Also, a comparison of our Fig. 7 and Fig. 4 of Ding \[36\] provides evidence that our non–square 16–site cluster has a momentum distribution function that behaves in a similar fashion to that found for the square $4 \times 4$ cluster.

The two hole ground state is a $\vec{k} = 0$ state (which was found in the subspace of zero total magnetization), and as Fig. 8 shows, the occupied electron states are within the antiferromagnetic Brillouin zone except for states at the wave vector of the one hole ground states, i.e. $\vec{k} = \pm(\frac{\pi}{2}, \frac{\pi}{2})$. Now, unlike the one hole ground state, only holes occupy these states. This is precisely the distribution function that one would expect based on rigid band filling arguments: the minimum energy states for one hole are at $\vec{k} = \pm(\frac{\pi}{2}, \frac{\pi}{2})$, and now for two holes both of these states are occupied by holes. Also, this is a very different conclusion from
that reached by Stephan and Horsch [35] whose results on a twenty site lattice suggested that the single hole problem had little to do with the many hole ground state. This may be understood in part because for their lattice the important $\pm(\frac{\pi}{2}, \pm\frac{\pi}{2})$ states are not present - see the discussion in §VI.

We have used a small negative $t'$ to lift the unphysical one hole degeneracies, and it is these degeneracies that caused the difference between our results, shown in Fig. 8, and those of Ding [36], for two holes; this is a further example of the usefulness of including $t'$. Ding found that the $t - J$ two hole ground state was degenerate at $\vec{k} = (0, 0), \pm(\pi, 0)$, and $\pm(0, \pi)$ for the square $4 \times 4$ lattice. The inclusion of a small negative $t'$ lifts this degeneracy and makes the ground state a $\vec{k} = 0$ state. Then, an analysis of the electron and hole distribution function clearly shows the occupation of the $\pm(\frac{\pi}{2}, \pm\frac{\pi}{2})$ states, consistent with rigid band filling. This is to be compared with the occupation of the $\pm(\pi, 0), \pm(0, \pi)$ states that Ding found in his $\vec{k} = 0, t' = 0$ ground state.

The three hole ground state (which was again found in the subspace of the total magnetization being $\frac{1}{2}\hat{z}$) is at $\vec{k} = \pm(\frac{\pi}{2}, -\frac{\pi}{2})$, and the electron and hole distribution functions are shown in Fig. 9. In comparison to the two hole case, we now see that the third hole occupies the same momentum state as the crystal momentum of the ground state, while the first two holes are still found to occupy the $\pm(\frac{\pi}{2}, \frac{\pi}{2})$ states. This is again consistent with rigid band filling. To display this we have provided the minimum energy states for one hole in the $t - t' - J$ model in Table I. Note that the first excited state within the antiferromagnetic Brillouin zone is at $\vec{k} = \pm(\frac{\pi}{2}, -\frac{\pi}{2})$, and is thus the state that one would expect the third hole to occupy. Figure 9 is a vivid demonstration of the hole pockets that one would expect from rigid band filling arguments.

The four hole ground state (which was found in the subspace of zero magnetization) is a $\vec{k} = 0$ state. It has electron and momentum distribution functions, as displayed in Fig. 10, very similar in character to those of the fewer hole states. Hole pockets around the four momenta $\pm(\frac{\pi}{2}, \pm\frac{\pi}{2})$ are clearly in evidence; some small tendency towards an expansion of the pockets to form a closed fermi surface may be seen. This is consistent with the assumption
that the band structure around the antiferromagnetic zone faces is very flat along the zone boundary, but steep towards the $\vec{k} = 0$ point. These results are also suggestive of a crossover from hole pocket states to a Luttinger liquid [38], although this simple set of data from a finite cluster can in no way be considered to conclusively answer such an important question.

VI. DISCUSSION:

We have suggested the use of a non-square 16-site cluster which includes all the important reciprocal lattice points for the one hole problem, and lifts certain unphysical degeneracies. We have shown that no anomalous results are found for this cluster, and have doped it with a small number of holes. The magnetic structure factor clearly shows the movement of its peak with carrier density reminiscent of an incommensurate phase. Since we are only working with a finite cluster, and are incapable of doing a finite scaling analysis with these results, we cannot be sure whether these correlations survive in the bulk limit, but experiments suggest that only dynamical (i.e. short-ranged) correlations remain. We will present the dynamic structure factor for this model in a future publication, and this will allow for a more direct comparison with experiment.

We have studied the electron and hole distribution functions for the many hole problem. They provide clear evidence of the development of hole pockets near the ground state wave vectors of the one hole problem; as the doping increases it seems quite possible that the hole pockets disappear, and a Fermi surface obeying Luttinger’s theorem results. On the basis of an assumption of (i) the strong coupling limit, (ii) the one hole ground state’s character, viz. that it is a $\vec{k} = \pm(\frac{\pi}{2}, \pm\frac{\pi}{2})$ state producing long-ranged dipolar spin distortions, and (iii) the existence of such hole pockets, Shraiman and Siggia [3] proposed the presence of an incommensurate spiral phase - our results strongly support their theory.

Our results contrast with earlier studies of these same questions. Firstly, Moreo et al. [14] did not find robust evidence of incommensurability when the doping level of a square
4 × 4 cluster described by the $t − J$ model. Our Fig. 5 seem to be very direct evidence of such an underlying instability. In contrast to our use of $S(\vec{q})$, Dagotto et al. [39] has used the dynamic structure factor for a variety of hole fillings, and did not find any evidence of incommensurability. Clearly, our use of a cluster that includes all of the important reciprocal lattice vectors, and a high density of $\vec{k}$ points around the antiferromagnetic wave vector, has allowed us to make a more direct study of this problem.

The work of Stephan and Horsch [35] has been considered by some [40] to have clearly demonstrated that the single hole problem has nothing to do with the higher doping levels of interest. To be specific, their two hole work showed a Luttinger Liquid with a clear Fermi surface, and no hint of hole pockets. Their work was conducted on a number of different clusters. Our work brings into question the absoluteness of these conclusions - we have clear evidence of hole pockets, and a knowledge of the single hole ground and excited states are found to be all that is necessary to predict the behaviour of the single particle momentum distribution functions for many holes. Thus, the question that must be answered is: how can two studies using the same technique (exact diagonalization) produce such totally different conclusions? We feel that because our cluster has the important $\vec{k} = \pm(\frac{\pi}{2}, \pm\frac{\pi}{2})$ momentum states, and it is these states that are required to properly incorporate the dipole–dipole interactions associated with the spiral instability of Shraiman and Siggia [6], and, we do indeed find an incommensurability in these ground states, consistent with experiment, differing clusters lead to different hole–hole interactions, and these interactions must strongly depend on the momentum states that the holes occupy.

To emphasize this latter point, we note that the work of Ding [36] led him to conclude that some form of rigid band filling did indeed occur for two holes. He, however, thought that the two single particle states that combined to produce the two hole ground state were $\vec{k} = \pm(\pi, 0), \pm(0, \pi)$ states - no hole pockets are then produced. We found that when the unphysical degeneracy of these reciprocal lattice points and those at the faces of the antiferromagnetic Brillouin zone are lifted (using a small negative $t'$), and thus a different form of rigid band filling, one displaying hole pockets, is produced. This is again an example
of the strong dependence of the hole–hole interactions on the underlying single hole ground
and first few excited states, and the subsequent character of the many hole ground states.

Our results are clearly in support of some form of rigid band filling (e.g., see Fig. 10),
and thus suggest that knowledge gained from the study of the simpler one hole problem can
(sometimes) be used to understand instabilities occurring at higher carrier densities; e.g.,
the incommensurate spiral phase \[\text{(H)}\]. This is similar to conclusions reached previously by
one of us for the very weakly doped insulator \[\text{(23–27)}\], and lends credence to studies of other
aspects of this problem, e.g. transport in the normal state, that were based on an assumption
of rigid band filling \[\text{(11)}\] having begun with a strong–coupling description of doped \(CuO_2\)
planes.

ACKNOWLEDGEMENTS:

We wish to thank T. Barnes, T. Mason, S. Trugman, and especially A.M.S. Tremblay
for helpful comments. This work was supported by the NSERC of Canada.
REFERENCES

[1] S.–W. Cheong, *et al.*, Phys. Rev. Lett. **67**, 1791 (1991).

[2] T.E. Mason, *et al.*, Phys. Rev. Lett. **68**, 1414 (1992); (preprint).

[3] T.R. Thurston, *et al.*, Phys. Rev. B **46**, 9128 (1992).

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

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

[6] B.I. Shraiman, and E.D. Siggia, Phys. Rev. Lett. **62**, 1564 (1989).

[7] J. Zaanen, and O. Gunnarson, Phys. Rev. B **40**, 7391 (1989).

[8] C.L. Kane, *et al.*, Phys. Rev. B **41**, 2653 (1990).

[9] A. Singh, and Z. Tesanovic, Phys. Rev. B **41**, 614 (1990).

[10] H.J Schulz, Phys. Rev. Lett. **64**, 1445 (1990); ibid **65**, 2462 (1990).

[11] M. Inui, and P.B. Littlewood, Phys. Rev. B **44**, 4415 (1991).

[12] E. Dagotto, Int’l J. Phys B **5**, 907 (1991).

[13] D. Poilblanc, *et al.*, Phys. Rev. B **46**, 6435 (1992).

[14] A. Moreo, *et al.*, Phys. Rev. B **42**, 6283 (1990).

[15] S.A. Trugman, Phys. Rev. B **41**, 892 (1990).

[16] B.I. Shraiman, and E.D. Siggia, Phys. Rev. Lett. **61**, 1234 (1988).

[17] C.L. Kane, P.A. Lee, and N. Read, Phys. Rev. B **39**, 6880 (1989).

[18] R. Liu, *et al.*, Phys. Rev. B **46**, 11,056 (1992).

[19] K.J. Szczepanski, T.M. Rice, and F.C. Zhang, Europhys. Lett. **8**, 797 (1989).

[20] K.M. Rabe, and R.N. Bhatt, J. Appl. Phys. **69**, 4508 (1991).
[21] R.J. Gooding, Phys. Rev. Lett. 66, 2266 (1991).

[22] A. Aharony, et al., Phys. Rev. Lett. 60, 1330 (1988).

[23] B. Keimer, et al., Phys. Rev. B 46, 14,034 (1992).

[24] R.J. Gooding, and A. Mailhot, Phys. Rev. B 44, 11,852 (1991).

[25] R.J. Gooding, and A. Mailhot, Phys. Rev. B, Sept. 1, 1993.

[26] F.C. Chou, et al., submitted to Phys. Rev. Lett.

[27] R.J. Gooding, N. Salem, and A. Mailhot, in preparation.

[28] D.M. Frenkel, et al., Phys. Rev. B. 41, 350 (1990).

[29] P.W. Leung, and P.E. Oppenheimer, Comp. in Phys. 6, 603 (1992).

[30] P.B. Littlewood, et al. (preprint).

[31] H.J. Schultz, and T. Ziman, Europhys. Lett. 18, 355, (1992).

[32] M.S. Hybertsen, E.B. Stechel, M. Schlueter, and D.R. Jennison, Phys. Rev. B 42, 6268 (1990).

[33] R.J. Gooding, and V. Elser, Phys. Rev. B 41 2557, (1990).

[34] B.S. Shastry, Phys. Rev. Lett. 63, 1288 (1989).

[35] W. Stephan, and P. Horsch, Phys. Rev. Lett. 66, 2258 (1991).

[36] H.–Q. Ding, Physica C 203, 91 (1992).

[37] One caveat to choosing this value of $t'$ is that the incommensurability found in the magnetic structure factor is lost in that now the 3 hole ground state peaks at the antiferromagnetic wave vector. However, at $\vec{q} = (\frac{3\pi}{4}, \frac{3\pi}{4})$ the magnetic structure factor is only 1% less than it is at $(\pi, \pi)$; we do not consider this to have compromised our results. In fact, one can use a smaller $|t'|$, lift the unphysical 3 hole degeneracy, maintain
the incommensurability found in \( S(\vec{q}) \), but the 2 and 4 hole ground states are not \( \vec{k} = 0 \) states. Thus, we have used a value of the second near neighbour hopping that produces this latter result. Using a smaller \(|t'|\) does not change our results for the momentum distribution functions.

[38] J.M. Luttinger, Phys. Rev. 119, 1153 (1960); ibid, Phys. Rev. 121, 942 (1961); J.M. Luttinger and J.C. Ward, Phys. Rev. 118, 1417 (1960).

[39] E. Dagotto, et al., Phys. Rev. B 45, 10741, (1992).

[40] P. Horsch, and W. Stephan, p. 241 in “Electronic Properties and Mechanisms of High \( T_c \) Superconductors”, ed. by T. Oguchi, K. Kadowaki, and T. Sasaki (Elsevier, New York, 1992); in particular, see the discussion section that follows this presentation.

[41] S.A. Trugman, Phys. Rev. Lett. 65, 500 (1990).
FIGURES

FIG. 1. The 32–site cluster; the rectangle outlines the non–square 16–site cluster that we focus
on in this paper; this cluster is seen to be half of the 32–site cluster.

FIG. 2. Reciprocal lattice vectors for (a) the 32–site cluster, and (b) our non–square 16–site
cluster.

FIG. 3. A comparison of the magnetic structure factor for the undoped square 4 × 4 16–site, our
non–square 16–site, and the square 32–site, clusters. The reciprocal lattice points are as follows:
\( \Gamma = (0, 0) \), \( X = (\pi, 0) \), and \( M = (\pi, \pi) \).

FIG. 4. Band structures for one hole in the 4 × 4 and non–square 16–site clusters; we have used
\( t = 1 \) and \( J = .4 \).

FIG. 5. Magnetic structure factors for one, two, three, and four holes for the \( t – J \) model on
the non–square 16–site cluster.

FIG. 6. Magnetic structure factors for one, two, three, and four holes for the \( t – t' – J \) model
on the non–square 16–site cluster, with \( t'/t = .2 \).

FIG. 7. Distribution functions for (a) electrons, and (b) holes, for the single hole problem. The
ground state is degenerate at \( \vec{k} = \pm(\frac{\pi}{2}, \frac{\pi}{2}) \), and here we show the distribution functions for the
\( k = (-\frac{\pi}{2}, -\frac{\pi}{2}) \) state. The upper (lower) numbers represent the spin up (down) components. The
energy parameters of the \( t – t' – J \) model are \( t = 1, t' = -.1 \), and \( J = .4 \). The square outlines the
antiferromagnetic Brillouin zone.

FIG. 8. Distribution functions for electrons and holes, for the two hole problem. The ground
state is a \( \vec{k} = 0 \) state. The upper (lower) numbers represent the electrons (holes).

FIG. 9. Distribution functions for (a) electrons, and (b) holes, for the three hole problem. The
ground state is degenerate at \( \vec{k} = \pm(\frac{\pi}{2}, -\frac{\pi}{2}) \), and here we show the distribution functions for the
\( k = (\frac{\pi}{2}, -\frac{\pi}{2}) \) state. The upper (lower) numbers represent the spin up (down) components.
FIG. 10. Distribution functions for electrons and holes, for the four hole problem. The ground state is a $\vec{k} = 0$ state. The upper (lower) numbers represent the electrons (holes).