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1989 J. Phys.: Condens. Matter 1 891

(http://iopscience.iop.org/0953-8984/1/5/005)

J. Phys.: Condens. Matter **1** (1989) 891–900. Printed in the UK

Holes in finite electron systems with strong correlation

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Received 16 August 1988

Abstract. The ground-state properties of several finite two-dimensional clusters were numerically investigated within the Hubbard model. In particular the spatial distribution of holes (with respect to the half-filled band case) is studied in detail. It is found that in systems with frustrated sites the holes prefer to occupy these sites for large U, and repel each other. This effect can be used to stabilise the antiferromagnetic order in the clusters by introducing coupling to additional sites.

1. Introduction

One-dimensional and two-dimensional strongly correlated electronic systems have already been extensively studied, mainly as a model for the magnetic properties of solids. The recently discovered superconductivity in materials of the type La_2CuO_4 or YBa_2CuO_{7-x} has renewed interest in the two-dimensional Hubbard models, since it is generally believed that this phenomenon is probably a result of a direct (non-phonon mediated) interaction between electrons that are placed on a two-dimensional lattice. Many experimental results (Batlogg *et al* 1987, Bourne *et al* 1987, Leary *et al* 1987, Birgeneau *et al* 1987, Shirane *et al* 1987) suggest that models of this type may describe at least some important aspects of the high-T_c superconductivity. In several of these models non half-filled band cases were examined and holes were considered as the charge carriers (Huang and Manousakis 1987, Schrieffer *et al* 1988). Although we do not intend to study in detail a possible superconducting state in such systems, we will, however, examine the influence of holes on the spin structure of the ground state of a Hubbard lattice.

Since there are only a few known analytic results for the infinite two-dimensional Hubbard lattice, several studies have been conducted on small systems with a limited number of sites with the hope that from these results one can obtain some insight into the infinite system. Both exact diagonalisation methods and variational techniques were used in these studies and several interesting results were obtained (Kawabata 1979, Hirsch 1985, Callaway *et al* 1987, Callaway 1987, Sano and Takano 1987, Hirsch *et al* 1988, Pesch *et al* 1988). Following this idea we have investigated finite clusters with different geometries and various numbers of electrons in order to determine the magnetic properties of their ground state.

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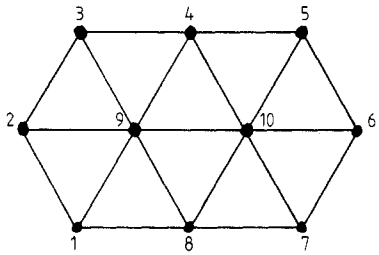

Figure 1. The ten-site cluster that is studied in § 2.

The Hamiltonian for the two-dimensional Hubbard model generally has the following form if nearest-neighbour and higher interactions are neglected.

$$H = t \sum_{\substack{\sigma,l \\ k(\mathrm{NN})}} c^{\dagger}_{l,\sigma} c_{k,\sigma} + U \sum_{l} n_{l\uparrow} n_{l\downarrow} . \tag{1}$$

The creation of holes in the half-filled band system can critically influence the ground-state properties of the Hubbard lattice. As an example we refer to the result of Nagaoka (1968), who has proved that if only one hole exists in a lattice with no frustration, its ground state is ferromagnetic for large U. In contrast to this, in the half-filled band case the Hamiltonian for large U can be mapped to the Heisenberg model, so the ground state is antiferromagnetic. For these reasons we made a thorough investigation of the properties of holes in both the triangular and the square lattices. Finite clusters with these structures were studied by exact diagonalisation of the exact Hamiltonian (1), or of the approximate Hamiltonian valid for large U, which was proposed in Harris and Lange (1967).

In § 2 we present results concerning a cluster with ten sites and eight electrons (or two holes). This cluster is a section of a triangular lattice, and its half-filled band case has been studied in our previous work (Mistriotis *et al* 1988). In § 3 we present the approximate Hamiltonian proposed in Harris and Lange (1967), and discuss its range of validity. Finally, in § 4 we present results concerning a section of a square lattice with eleven sites and ten electrons (one hole). In this model we particularly study the influence on the ground state of an extra site lying outside the plane of the square lattice, which is connected to one or two sites of the main cluster. This extra site can stabilise the antiferromagnetic order for large U, because it causes localisation of the hole for certain values of the bond strength.

2. A finite triangular lattice

In this section we present results for a ten-site cluster (figure 1), which is a section of a triangular lattice, and some of its properties have already been studied in Mistriotis *et al* (1988). This cluster has sites with different coordination number, so here we examine to what extent this fact can influence the position of a hole, or the distance between two holes in the ground state of the system.

We diagonalised the exact Hamiltonian (1) for this cluster with eight electrons (two holes). Even though the maximum number of states was 44100, the corresponding

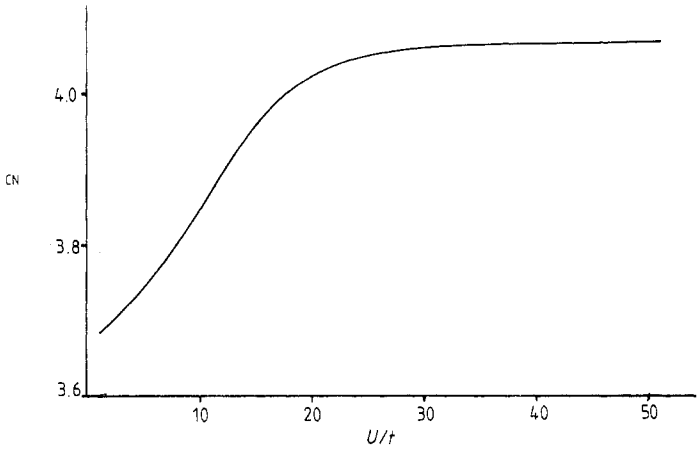

Figure 2. The average coordination number, CN, for the holes as a function of U/t for the cluster of figure 1 with eight electrons.

Table 1. Energy eigenvalues and eigenvectors of the one-particle system for the ten-site cluster. None of the states is degenerate. The number of sites is the same as in figure 1.

	Eigenvector for site No:									
Eigenvalue	1	2	3	4	5	6	7	8	9	10
−2.1730	−0.259	0.342	−0.259	0.446	−0.259	0.342	−0.259	0.446	−0.225	−0.225
−2	0.289	0	0.289	0	−0.289	0	−0.289	0	−0.577	0.577
−1.4142	−0.354	0	0.354	−0.500	0.354	0	−0.354	0.500	0	0
−1.3028	0.245	−0.565	0.245	0	−0.245	0.565	−0.245	0	0.245	−0.245
−1.1393	−0.317	0.152	−0.317	−0.252	−0.317	0.152	−0.317	−0.252	0.460	0.460
0	−0.500	0	0.500	0	−0.500	0	0.500	0	0	0
0.1963	0.143	0.553	0.143	−0.349	0.143	0.553	0.143	−0.349	−0.177	−0.177
1.4142	−0.354	0	0.354	0.500	0.354	0	−0.354	−0.500	0	0
2.3028	−0.326	−0.425	−0.326	0	0.326	0.425	0.326	0	−0.326	0.326
4.1160	0.249	0.231	0.249	0.341	0.249	0.231	0.249	0.341	0.453	0.453

matrix was diagonalised successfully by the Lanczos method in relatively short computing time. Both the average coordination number of holes, and the average distance between two holes in the ground state were calculated as a function of the interaction energy U/t.

More specifically, figure 2 shows that the average coordination number of a hole increases with U. In other words the holes prefer to be in the two central sites of the cluster, where the coordination number is 6. This behaviour is caused by the fact that the holes tend to occupy the highest state of the band of the corresponding non-interacting electron system, as U increases. The non-interacting electron Hamiltonian can be easily solved and the resulting eigenvalues and eigenvectors are presented in table 1. The eigenvector corresponding to the highest eigenstate shows that this state is indeed mainly localised at the sites with high coordination. This is to be expected, since

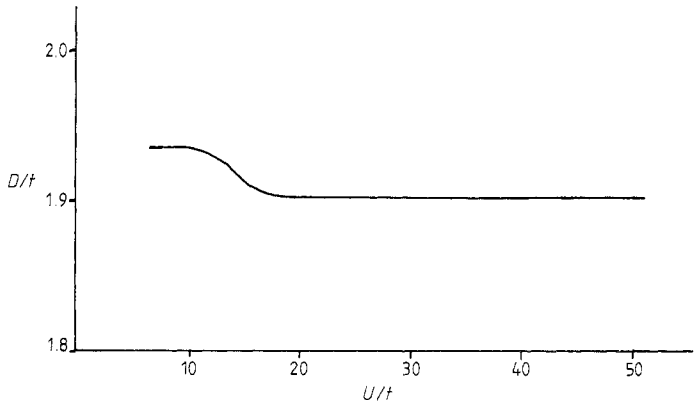

Figure 3. The average distance between the two holes, D/t, as a function of U/t for the cluster of figure 1 with eight electrons.

generally the highest and the lowest states of the corresponding one-particle system are most strongly influenced by the largest hopping probability in the cluster.

In figure 3 the average distance between two holes in the cluster is plotted as a function of U. We present results only for U larger than the one-particle bandwidth, because in this case there are no electron pairs in the ground state, so we have exactly two unoccupied sites in the system. Indeed no electron pairs can exist in the ground state if U is larger than the bandwidth, since any state with pairs has energy higher than the maximum spin state, where no pairs exist. For the examined cluster the bandwidth is equal to $6.2890t$, as table 1 shows.

Our results show a weak attraction between the two holes as U increases for a range of U-values between $7t$ and $50t$. In other words the average distance between the holes decreases in this region of U. Nevertheless, if U is further increased, the distance between the holes increases slightly again. More specifically the average distance between the two holes for $U = 1000t$ is 1.935, while for $U = 50t$ it is 1.905. This result is in agreement with what was found for the one-dimensional Hubbard lattice (Zotos 1988). Finally we note that the average distance between two holes when they are randomly placed on the cluster is only 1.733, which is substantially smaller than the value corresponding to large U. Therefore, an overall repulsion between the holes exists.

In § 4, we will examine the behaviour of holes also in a section of the square lattice with no frustration, but before doing that we present an approximate Hamiltonian, valid for large U, which drastically reduces the total number of states, and facilitates the computations.

3. The approximate Hamiltonian for large U

For large U we expect that no electron pairs can exist in the ground and the low-lying states of a Hubbard cluster. Therefore these low-lying states can be well determined if all states with pairs are projected out. This approximation yields the following effective

Hamiltonian (Harris and Lange 1967).

$$H_{\text{app}} = H_1 + H_2 + H_3$$

$$H_1 = -t \sum_{\substack{i,\sigma \\ j(\text{NN})}} c^{\dagger}_{i,\sigma} c_{j,\sigma}$$

$$H_2 = \frac{t^2}{U} \sum_{\substack{i \\ j(\text{NN})}} (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j - 1) \tag{2}$$

$$H_3 = -\frac{t^2}{U} \sum_{j,k(\text{NN})}^{i,\sigma} [(c^{\dagger}_{k,\sigma} c_{i,\sigma}) n_{i,-\sigma} (c^{\dagger}_{i,\sigma} c_{j,\sigma}) + (c^{\dagger}_{k,-\sigma} c_{i,-\sigma}) n_{i,-\sigma} (c^{\dagger}_{i,\sigma} c_{j,\sigma})].$$

If there are no holes in the system (half-filled band case), H_1 and H_3 vanish, and the Hamiltonian is mapped to a Heisenberg Hamiltonian, while for a finite number of holes and large U, only the term H_1 contributes significantly to the ground-state energy.

The above approximation, namely that no electron pairs exist in the ground state, should be valid for U larger than the non-interacting electron bandwidth. This is explained by the fact that the existence of a pair raises the ground-state energy by U, while the maximum energy needed for breaking a pair is equal to the non-interacting electron bandwidth. Moreover in Mistriotis *et al* (1988) we have shown numerically that the approximate Hamiltonian (2) gives quantitatively good results for values of U larger than approximately three times the bandwidth. In the next section, we use the above effective Hamiltonian to calculate the ground-state properties of a cluster with 11 sites.

4. A finite square lattice with an extra outer site

Models with strongly correlated electrons on a square lattice have been extensively studied recently, because this geometric structure corresponds to the CuO planes of the new superconducting materials. In this section we study a $\sqrt{10} \times \sqrt{10}$ unit cell, which was first proposed in Oitmaa and Betts (1978). This cluster, even though it is finite, has no frustration if periodic boundary conditions are applied. Therefore it is an appropriate model for studying the spin structure of the infinite lattice.

More specifically, we would like to study the influence of holes on the ground state of this cluster. Previous studies have shown that if a hole is introduced into the system (nearly half-filled band), a transition takes place as U increases for the ground state, which changes from an antiferromagnetically ordered state to one with local ferromagnetic order (Kaxiras and Manousakis 1988). This transition occurs for a value of U ($U \simeq 33$) slightly larger than the rate of validity of the effective Hamiltonian (2). Therefore it is an interesting question how the antiferromagnetic state can be stabilised in the presence of holes.

Our results of § 2 show that a hole is localised at sites where the hopping probability is large. Hence we examined the possibility that the influence of a hole on the spin structure of the cluster is reduced, when one or more sites in the square lattice cluster are connected to an extra site with additional bonds, having a hopping parameter $t_1 > t$.

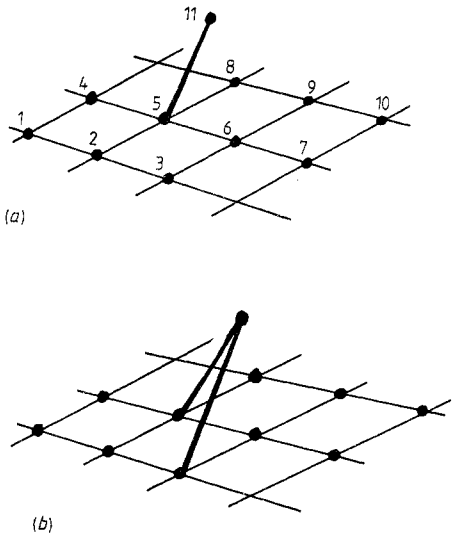

Figure 4. Square lattice clusters connected to an outer site by (*a*) one or (*b*) two bonds. These clusters are investigated in § 4.

We have therefore investigated the two clusters of figure 4, where the extra outer site is connected to one or two sites of the square lattice. The above clusters were studied by an exact diagonalisation of the matrix corresponding to the approximate Hamiltonian (2).

Before presenting our results it is necessary to determine the range of validity of the Hamiltonian (2) for the clusters of figure 4. In § 3, we explained that this approximation gives good quantitative results for the ground state if U is larger than about three times the one-particle bandwidth. The one-particle states for these two clusters can be determined analytically. If t is the energy unit, there are in both cases three eigenvalues equal to 1, three others equal to -1, and one equal to 0. The other four eigenvalues depend on t_1 and have the form

$$\varepsilon = \pm \{[t_1^2 + 17 \pm (t_1^4 - 18t_1^2 + 225)^{1/2}]/2\}^{1/2} \tag{3}$$

for the cluster of figure 4(*a*), where there is only one connection to the extra site, while for the cluster 4(*b*) they are given by

$$\varepsilon = \pm \{[2t_1^2 + 17 \pm (4t_1^4 - 12t_1^2 + 225)^{1/2}]/2\}^{1/2}. \tag{4}$$

Therefore the bandwidth can also be determined analytically. For all values of t_1 that we have examined, the bandwidth is smaller than 20. Hence the approximation that no pairs exist in the ground state is valid for $U \geqslant 20$. The value of U corresponding to three times the bandwidth, beyond which the results are considered to be also quantitatively accurate, is marked by a small vertical line in each curve of figure 5. In this figure we present the results for the following correlation function:

$$F = \sum_{\substack{k(\text{NN of } 1) \\ l(\text{NN of } 6)}} \langle (n_{1\uparrow} - n_{1\downarrow})(n_{k\uparrow} - n_{k\downarrow}) \rangle + \langle (n_{6\uparrow} - n_{6\downarrow})(n_{l\uparrow} - n_{l\downarrow}) \rangle. \tag{5}$$

This correlation is negative for antiferromagnetic order on the square lattice plane. Furthermore, we calculated the degree of localisation of the hole, in other words the

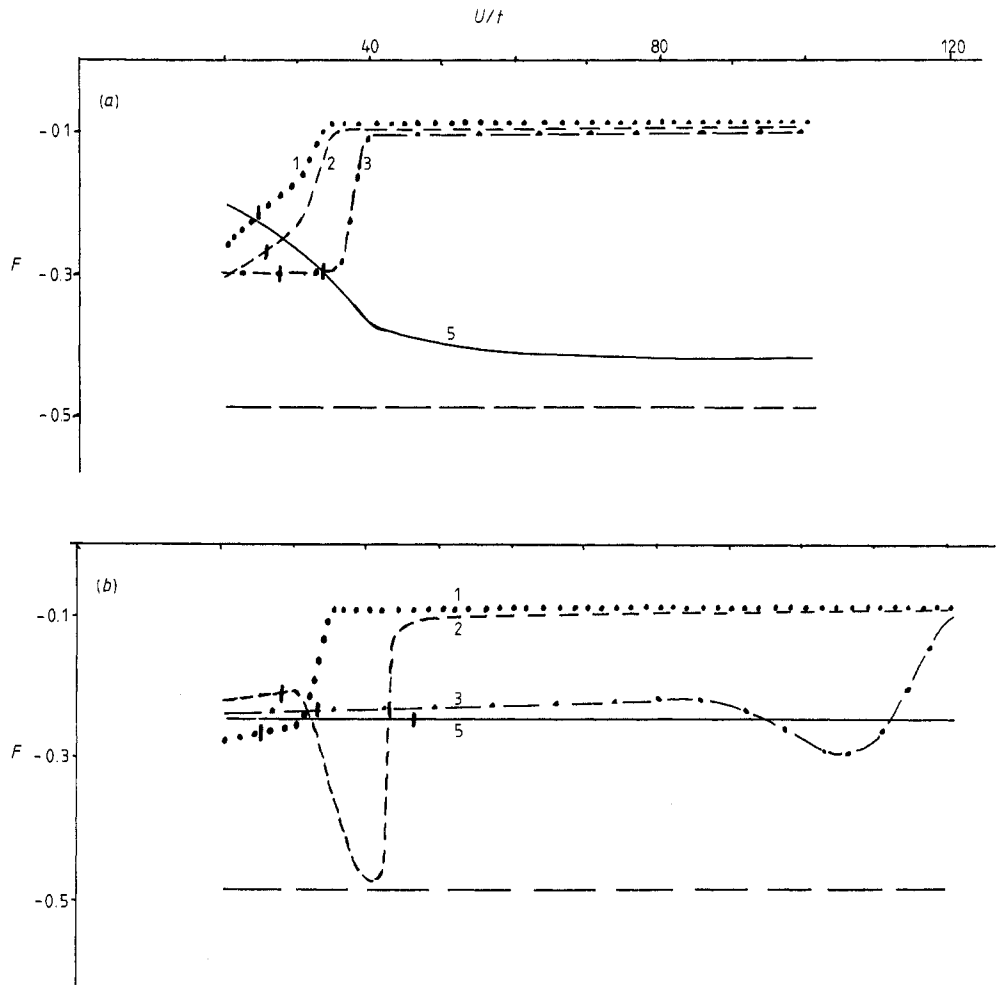

Figure 5. The correlation function F for the clusters of (a) figure 4(a) and (b) figure 4(b) with ten electrons as a function of U/t. The numbers on the curves correspond to the value of the hopping parameter t_1/t of the extra bonds. The broken horizontal line shows the value of the correlation function F for the square lattice cluster without the outer site with ten particles (half-filled band case). The small vertical marks indicate the values U/t, equal to three times the bandwidth of the non-interacting electron system.

probability P that the hole lies in the outer site. These results are presented in figure 6.

Figures 5(a) and (b) show the behaviour of correlation (5) as a function of U for the clusters of figures 4(a) and (b) respectively, while t_1 takes the values 1, 2, 3, and 5. The broken horizontal line on these figures shows the value of the same correlation function (5) corresponding to the half-filled band case of the ten-site cluster without the extra outer site. This value which is obtained by solving the corresponding Heisenberg model, can be used as a reference to check whether the antiferromagnetic order is preserved.

Our results show that in the case where the extra site is connected to only one site on the plane, a transition from an antiferromagnetic state ($S = 0$) to a state with large total spin ($S = 4$) takes place as U increases, similarly to the transition that was observed for

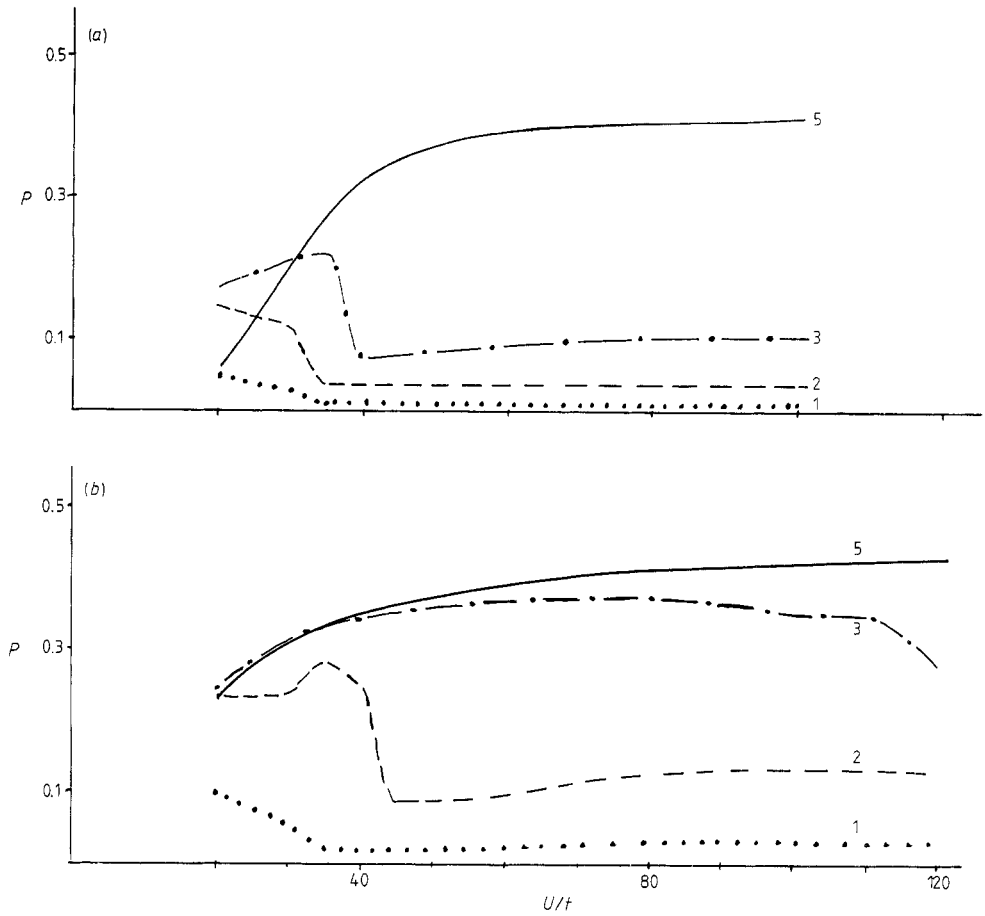

Figure 6. The degree of localisation, P, of the hole at the outer site for the clusters of (*a*) figure 4(*a*) and (*b*) figure 4(*b*) with ten electrons as a function of U/t. The numbers correspond to the value of the hopping parameter t_1/t of the extra bonds.

the cluster without the outer site. The critical value of U where this transition occurs increases with t_1. Particularly for $t_1 = 5$, the antiferromagnetic order of the ground state is preserved for values of U as large as 100, although it is finally destroyed for very large U ($\simeq$500). This behaviour can be understood as a result of the localisation of the hole at the outer site, which reduces its influence on the spin structure of the ground state. Indeed, as figure 6(*a*) shows, the probability P that the hole lies in the extra outer site exhibits a transition at the same values of U where the transition for the correlation function (5) takes place.

Similar behaviour is also observed when the extra site is connected to two sites on the plane. Even though the existence of two bonds instead of one slightly changes the ground state properties, a transition from a small total spin state ($S = 1$) to the maximum spin ($S = 5$) state occurs. For this cluster, the antiferromagnetic order is also preserved for a range of U-values that increases with t_1, but the antiferromagnetic correlation is weaker. Nevertheless a strongly antiferromagnetic ground state exists for some com-

binations of U and t_1, as figure 5(b) shows. For example if $t_1 = 2$ and $U \simeq 40$ the value of the correlation function (5) is similar to that of the Heisenberg model. Figure 6(b) also shows that for this cluster, the reason for preserving the antiferromagnetic character of the ground state is the localisation of the hole at the extra outer site.

Therefore, the existence of sites that lie outside the plane of a square lattice, and the type of bonding with sites on the plane can critically influence the properties of the ground state of the system. Note that if a second hole is introduced to the above clusters the value of the correlation function (5) becomes zero for all the values of U larger than 20.

5. Conclusions

In this investigation we have described two main results which are conjectured to be also true for larger two-dimensional systems.

(i) In lattices with frustrated sites the holes tend to occupy these sites. Moreover if two holes exist in the lattice, there is a net repulsion between them. In other words the average distance between the two holes is larger than the average distance between two holes randomly placed on the system.

(ii) Additional sites outside a square lattice connected to the main plane by a hopping parameter $t_1 > t$, tend to trap holes for large values of U. As a result the influence of the holes on the main square lattice is reduced, and the antiferromagnetic order in the plane is stabilised.

These interesting points should be further investigated in larger systems because they may be also relevant to high-T_c superconductivity.

Acknowledgments

This work was partly supported by the European Stimulation Program (Contract No ST2J-0032-3-D (CD)).

References

Batlogg B *et al* 1987 *Phys. Rev. Lett.* **58** 2333
Birgeneau R J *et al* 1987 *Phys. Rev. Lett.* **59** 1329
Bourne L C, Corommie M L, Zettel A, zur Loye H C, Keller S W, Leary K L, Stacy A M, Chang K J, Cohen M L and Morris D E 1987 *Phys. Rev. Lett.* **58** 2337
Callaway J 1987 *Phys. Rev.* B **35** 8723
Callaway J, Chen D P and Tang R 1987 *Phys. Rev.* B **35** 3705
Harris A B and Lange R V 1967 *Phys. Rev.* **157** 295
Hirsch J E 1985 *Phys. Rev.* B **31** 4403
Hirsch J E, Tang S, Loh E and Scalapino D J 1988 *Phys. Rev. Lett.* **60** 1668
Huang K and Manousakis E 1987 *Phys. Rev.* B **36** 8302
Kawabata A 1979 *Solid State Commun.* **32** 893
Kaxiras E and Manousakis E 1988 *Phys. Rev.* B **37** 656
Leary K J, Zur H-C and Stacy M 1987 *Phys. Rev. Lett.* **59** 1236
Mistriotis A, Büttner H and Pesch W 1988 *J. Phys. C: Solid State Phys.* **21** L1021
Nagaoka Y 1968 *Phys. Rev.* **147** 392

Oitmaa J and Betts D D 1978 *Can. J. Phys.* **56** 897
Pesch W, Büttner H and Reichl J 1988 *Phys. Rev.* B **37** 5887
Sano K and Takano K 1987 *J. Phys. Soc. Japan* **56** 4229
Schrieffer J R, Wen X-G and Zhang S-C 1988 *Phys. Rev. Lett.* **60** 944
Shirane G, Endoh Y, Birgeneau R J, Kastner M A, Hidaka Y, Oda M, Suzuki M and Murakami T 1987 *Phys. Rev. Lett.* **59** 1613
Zotos X 1988 *Phys. Rev.* B **37** 5594