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Numerical studies of Hubbard clusters: exact diagonalization and Monte-Carlo simulation

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Abstract We present results of the exact diagonalization of the Hubbard model in clusters of 4,5 and 6 sites by increasing the prirnitive tetrahedral cell and obeying the f.c.c. lattice symmetries. Ground state properties such as the energy spectrum, the total spin of the cluster and spin pairing correlation functions have been calculated and a magnetic phase diagram is reported. We also present exact diagonalization and numerical simulation results for an almost one-dimenional system which, we believe, is the simplest periodic lattice to exhibit ferromagnetism in a half-filled band in agreement with a recent theorem by Lieb.

1. Introduction

Since its proposal[1] the Hubbard model has been used to describe the properties of narrow band itinerant electron systems[2], normal liquid ^3He and low dimensional conductors[4]. Extended versions of it have been of interest in studying one-dimensional organic semiconductors[5]. After the discovery of high-temperature superconductors much attention has been given to this model, both in the weak and strong coupling regimes[6].

In the simplest version of the single-band Hubbard model electrons can hop only between Wannier states of neighboring lattice sites and interact via a local Coulomb repulsion. The Hamiltonian is:

$$\mathcal{H} = -t\sum_{i,j,\sigma} c^{+}_{i\sigma}c_{j\sigma} + \frac{U}{2}\sum_{i\sigma} n_{i\sigma}n_{i-\sigma},$$

where t is the hopping integral between neighboring sites, U is the on-site Coulomb repulsion between eletrons of opposite spins, $c_{i\sigma}(c^{+}_{i\sigma})$ is the annihilation (creation) operator for fermions of spin σ on site i and $n_{i\sigma}$ is the electron number operator.

In spite of its apparent simplicity, the model cannot be solved exactly except in one-dimension[7] where the ground state has been proved to be antiferromagnetic and insulating for $U > 0$ and half-filled band. Recently, Kawakami et al[8] obtained the thermodynamic properties of the one-dimensional model by means of the Bethe Ansatz method, which are in excellent agreement with Shiba's[9] small cluster calculation. In the last few years, the two-dimensional Hubbard model has been extensively studied[6] because of its possible connection with high-temperature superconductivity. It has been found that an insulating antiferromagnetic state exists in the half-filled band case. The metallic and the superconducting states are under current investigation.

It is of interest to point out that in one and two dimensions the continuous spin symmetry of the model cannot be broken and, thus, no ferromagnetism is found at finite tmperatures. However, this is not true for the ground state. In fact, along the years the literature has accumulated plenty of controversy[10] concerning the possibility that the nondegenerate version of the model might exhibit, under any circumstance, a ferromagnetic ground-state, even in three dimensions[11]. Nagaoka[12] obtained, for the f.c.c. lattice with one hole in a half-filled band, a ferromagnetic solution in the infinite U limit. The validity of Nagaoka's argument for systems in the thermodynamic limit has, however, been questioned[10]. Very recently Lieb presented[13] the first provable example of itinerant-electron ferromagnetism, thus taking a significant step forward. He showed that a bipartite lattice with a half-filled nondegenerate band has ground-state spin$S = \frac{1}{2}||B| - |A||$, where $|B|(|A|)$ is the number of sites in the $B(A)$ sublattice. The theorem holds in all dimensions without even the need of a periodic lattice structure.

In this work we study ground state properties of the f.c.c. lattice through the exact diagonalization of clusters of 4 to 6 sites obtained by increasing the primitive tetrahedral cell. The clusters are treated as free: periodic boundary conditions are not imposed. In these systems, the absence of electron-hole symmetry hinders

the direct use of standard Monte Carlo simulation. Saturated ferromagnetism, unsaturated ferromagnetism and paramagnetism are found for certain values of U/t and n, where n is the average number of electrons per site. Our results for the tetrahedral cell reproduce those of Falicov and Victora[14] and the phase diagram compares well with others obtained using approximate bulk techniques[15,16].

We also introduce an almost one-dirnensional bipartite lattice and consider clusters of 6 and 9 sites in order to verify Lieb's theorem. The former was exactly diagonalized for various strengths of the Coulom repulsion, resulting in a $S = 1$ ground-state, because $|B| = 4$ and $|A| = 2$. The latter was simulated by Monte Carlo techniques with good indication of unsaturated ferromagnetism.

2. Ground-State Phase Diagram of the f.c.c. Hubbard Model

The single-particle energies for the f.c.c. tight-binding lattice are:

$$E_{\vec{k}} = t \sum_i e^{i\vec{k}.\vec{R}_i} = 4t[\cos(k_x/2\cos(k_y/2) + \cos(k_y/2)\cos(k_x/2) + \cos(k_x/2)\cos(k_z/2)], \quad (2)$$

where $\vec{k}$ is the wave vector in the first-Brillouin zone and $\vec{R}_i$ are the positions of the first neighbors of a lattice site. Another interesting feature of the noninteracting system is the density of states defined by:

$$\rho(E) = \sum_{\vec{k}} \delta(E - E_{\vec{k}}). \quad (3)$$

As one sees from its shape (Fig.1) the system does not display particle-hole symmetry and hence the chemical potential is not $U/2$ for a half-filled band, leading to negative Boltzmann weights[17]. The ground state is obtained by filling the states with lowest energies.

Our approach to consider electron correlations is based on exact numerical diagonalization of the clusters shown in Fig.2, obtained by increasing the tetrahedral cell and obeying the f.c.c. lattice symmetries, such as to maximize the number of bonds.

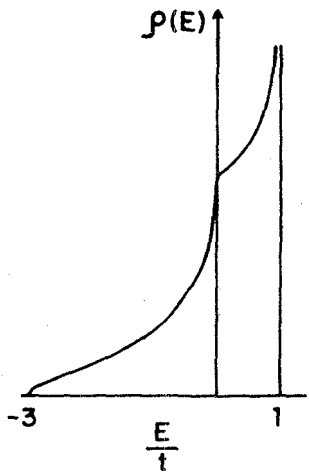

Fig. 1 – Band density of states for a tight-binding f.c.c. lattice.

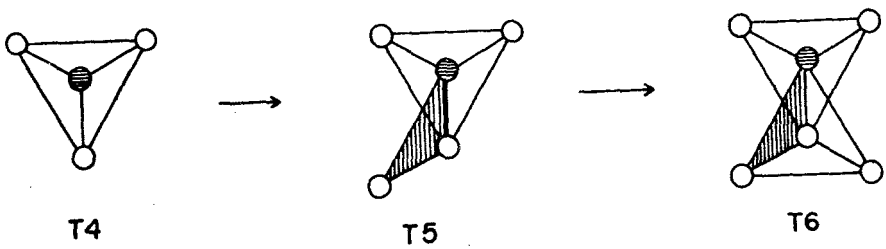

Fig. 2 – f.c.c. lattice clusters of 4,5 and 6 sites.

We treated the Hamiltonian (1) on a basis of states $|n_{i\sigma}>$ in which it is diagonal for the electron number operator. The results are valid for either positive or negative values of t and related through the identity:

$$E_{2Na-Ne}(-t) = E_{Ne}(t) + U \times (Na - Ne), \tag{4}$$

where $Na(Ne)$ is the number of atoms (electrons) of the cluster. In this way, the energy spectra have been calculated and typical reslts are shown in Fig.3 for the cluster ***T5*** with 7 electrons, for $U/t = 2$ and $U/t = 8$. The opening of a gap as U increases is the mechanism underlying the Mott metal-insulator transition in a half-filled band.

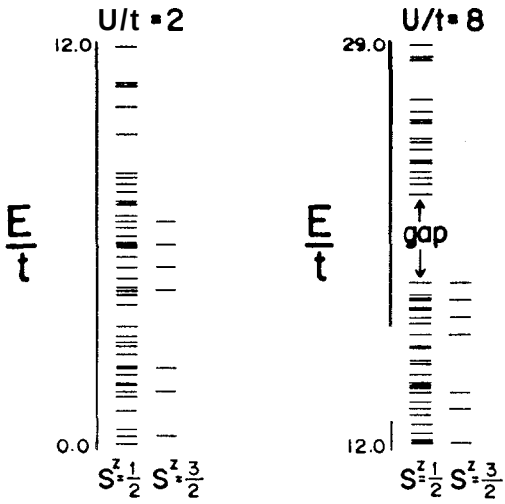

Fig. 3 - Energy spectra of an f.c.c. cluster of 5 sites with 7 electrons for $U/t = 2$ and $U/t = 8$.

The total spin of the ground-state for a specific set of parameter values can be pictured by filling the one-particle energies given in Fig.4. The diagrams in figures 5,6 and 7 show those cases for which ferromagnetism appears for some interval of values of $z = t/U$.

For the tetrahedron, the ground-state has maximum spin when $N_e = 5$ and the number of holes $N_h = 2N_a - N_e = 3$ [Fig.5(a)]. This configuration of maximum spin state is termed saturated ferromagnetism (SF). Notice that by changing $t \rightarrow -t$ the hole ground-state is obtained by placing three holes of parallel spins in the threefold degenerate level of energy $-t$. As the Coulomb repulsion term has no effect in this state, the ground-state energy and spin state are the same for all z. For $N_e = 6$ or $N_h = 2$ [Fig.5(b)- 5(c)] there is a degeneracy of the singlet and triplet spin states. For other values of the occupation number the state of minimum spin [Paramagnetism (P)] is preferred.

For the cluster T5 with 6 electrons (Fig.6) we have three possibilities: the singlet (S = 0), the triplet ($S = 1$) and the quintuplet ($S = 2$) spin states.

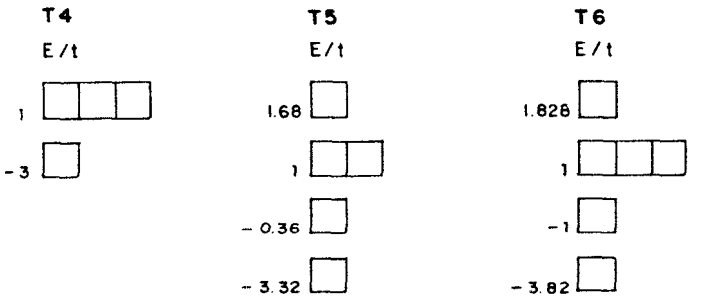

Fig. 4 – One-particle energy levels and degeneracies of f.c.c. clusters.

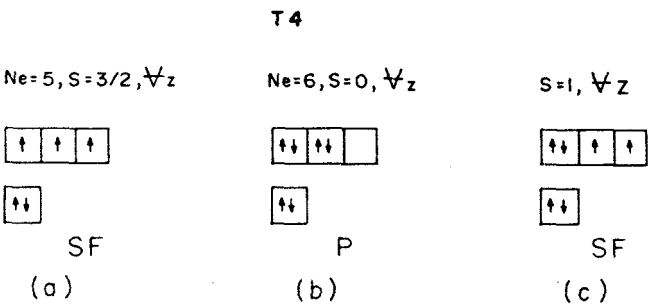

Fig. 5 – a. Configuration of maximum spin (SF) for the terahedral cluster with 5 electrons. b. Degeneracy of the singlet and triplet spin states for the tetrahedral cluster with 6 electrons.

The spin of the configuration increases with decreasing z since larger values of U inhibit the appearance of singlet spin states in the one-particle levels. The state with intermediate value of spin is called unsaturated ferromagnetism (USF). Other configurations for the cluster T5 with 7 electrons and for the cluster T6 with 7 and 8 electrons are shown in Fig. 6(d)-6(e) and Fig.7, respectively.

One should stress that in the above arguments using on-particle states the degeneracy of the levels played an important role for the occurrence of a ferromagnetic state, in analogy with the Stoner-type criterion for bulk systems in

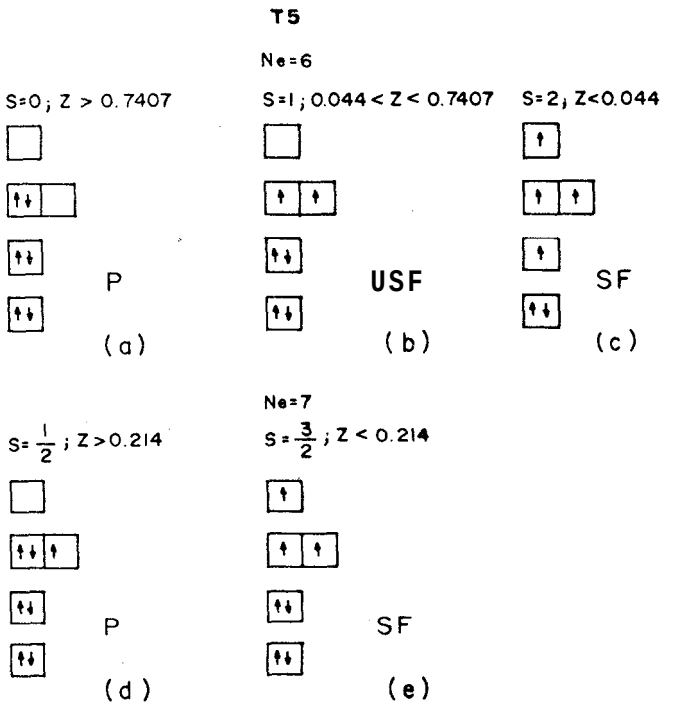

Fig. 6 – Paramagnetic [(a) and (d)], unsaturated ferromagnetic (b) and saturated ferromagnetic [(c) and (e)] configurations for the cluster T5 with 6 and 7 electrons.

which ferromagnetism is predicted if the Fermi levels lie near a peak in the density of states.

The results derived in this section are now used to draw a phase diagram $|t|/U$ x n (see Fig.8). The cases of positive and negative t reduce to each other by reflection. In analyzing the diagram we restrict ourselves to the case $t > 0$.

First, we should point out that *no* magnetic solutions occur until the band is *half-filled*, as in Nagaoka's analysis. The divergence at $n = 1.25$ divides the phase diagram into two parts. The first one, for $1 < n < 1.25$, in which a transition from SF to USF exists before the system enters the paramagnetic phase for a

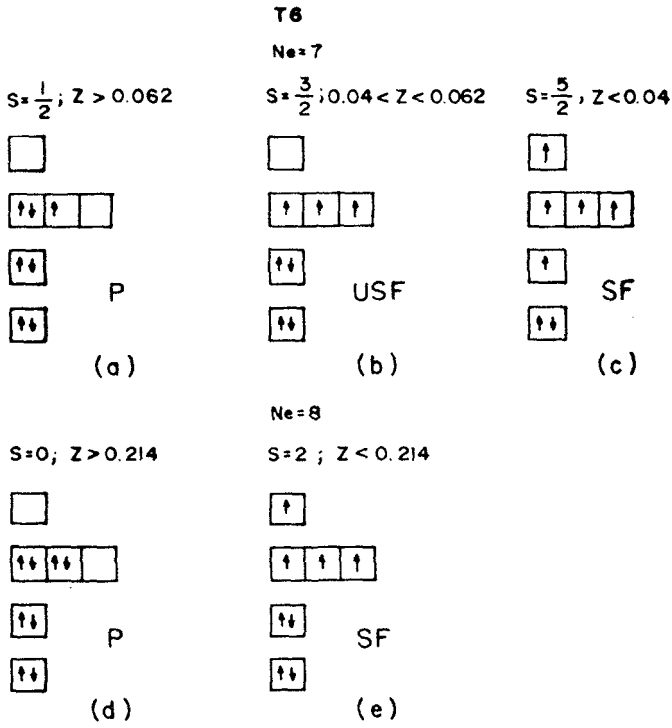

Fig. 7 – Same as Fig.6 for the cluster T6 with 7 and 8 electrons.

smaller value of U. This result is in agreement with the Meyer and Schweitzer's calculation[15] using Green's function techniques in the infinite U limit. In the second region, $1.25 < n < 1.5$, there is no USF phase. In bulk calculations[15], however, ferromagnetism is predicted all the way before the band is filled at $n = 2$. The insert in Fig. 8 compares our solution with that of Hashimoto[16] using a generalized Gutzwiller strong-coupling method. Though the results agree near half-filled band, ferrmagnetism is not found for $n < .5$ in our cluster calculation. In fact we do not expect the electronic correlations in bulk systems to be adequately described in a finite system in the regime of low hole ($t > 0$) or particle-($t < 0$) density. To illustrate this point consider the tetrahedron with one free electron,

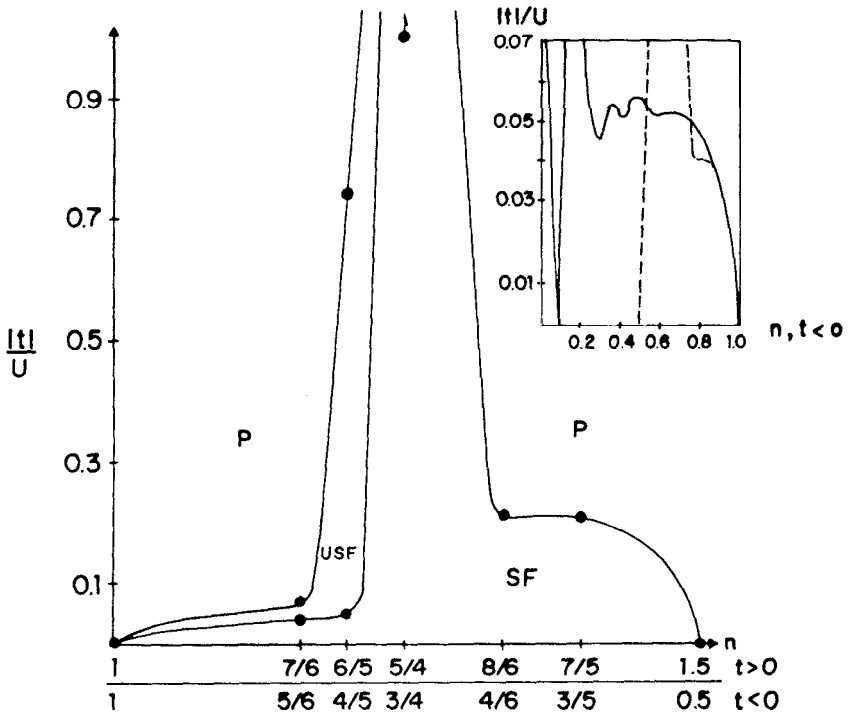

Fig. 8 – Ground state $|t|/U$ x n phase diagram for an f.c.c. lattice based on exact diagonalization of clusters of 4,5 and 6 sites, showing paramagnetic (P), unsaturated ferromagnetic (USF) and saturated ferromagnetic (SF) phases. The lines are guides to the eyes. The insert compares our result with the approximate bulk solution of Hashimoto (Ref.16).

i.e., n = .25. In the bulk the same band filling corresponds to a system with a large number of interacting electrons.

In order to better understand the characteristics of the SF and USF orderings, one can study the longitudinal spin correlation functions

$$L_\delta = \frac{1}{N_a}\sum_i < 0|S_i^z S_{i+\delta}^z|0 >, \qquad (5)$$

where $S_i^z = (1/2)(n_{i\uparrow} - n_{i\downarrow})$, | is the ground-state eigenvector, i labels the lattice sites and δ defines the order of neighborhood o the correlation function. L_0 mea-

sures the magnitude of the local moment whereas L_1 and L_2 test, respectively, the correlation between first- and second- neighbor local spins.

In Fig. 9 we plot the local moment, L_0, versus z. It decreases with increasing z, as the system evolves from the localized limit $(z = 0)$ to the iinerant one $(z = \infty)$, explicitly showing the breakdown of magnetic correlation. On the other hand, the results presented in Fig.10 show that $L_1, L_2 > 0$ in the SF phase, $L_1 > 0$ and $L_2 < 0$ in the USF phase and $L_1, L_2 < 0$ in the paramagnetic phase of the f.c.c. Hubbard clusters. Notice also that the correlation functions are discontinuous at every transition, and that evcn in the paramagnetic phase the system sustains some degree of magnetic correlation.

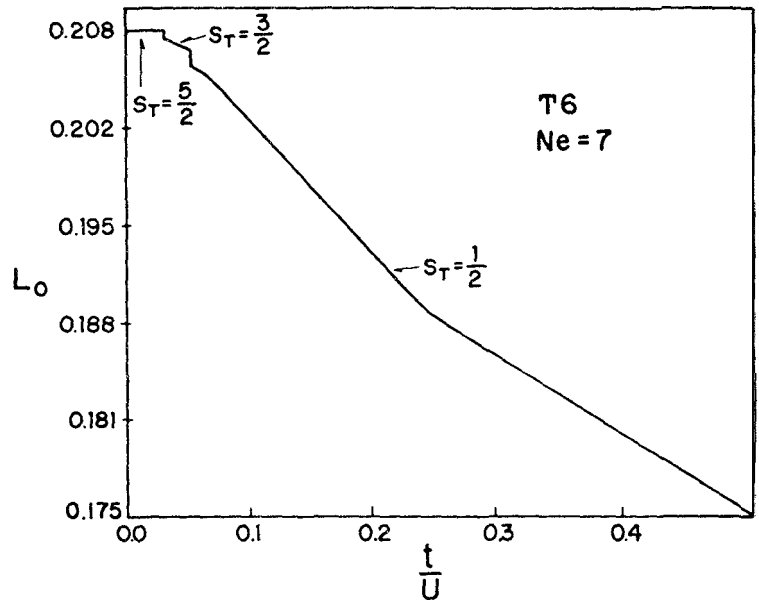

Fig. 9 – Local spin as a function of $z = t/U$ for an f.c.c. cluster of 6 sites and 7 electrons.

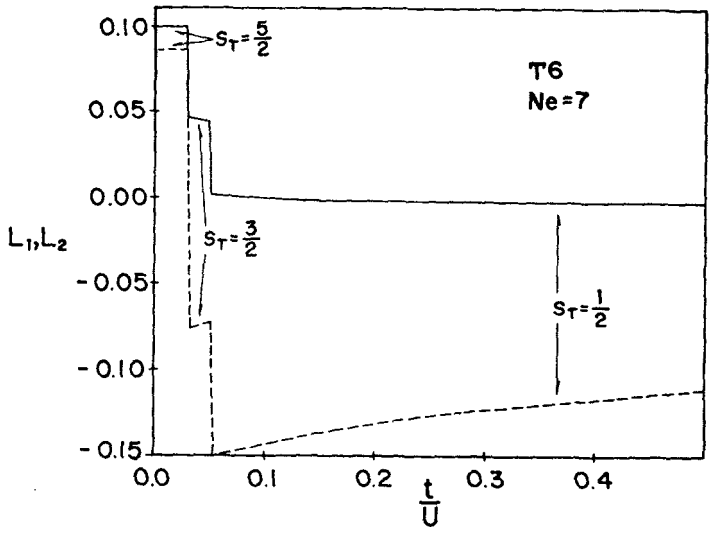

Fig. 10 – First (L_1 full line) - and second (L_2, dashed line) - neighbor spin correlation functions versus $z = t/U$ for an f.c.c. cluster of 6 sites and 7 electrons.

3. Monte Carlo Simulation and Lieb's Theorem

The purpose of this section is to verify a recent theorem by Lieb which proves the existence of ferromagnetism in a *half-filled* bipartite lattice with distinct numbers of sublattice sites in the unit cell. In Fig.11 we sketch an almost one-dimensional system with periodic boundary conditions. Hopping occurs only between first-neighbors sites of sublattices A and B. We believe this is the simplest periodic lattice to satisfy Lieb's theorem. Since each unit cell has 2 atoms on sublattice B and one on A, a net one-half spin should survive.

We have checked the above predictions by exact diagonalization of a cluster of 6 atoms and found that the ground state is indeed ferromagnetic with total spin S = 1 for all values of U/t. We have also performed quantum Monte Carlo simulations for a cluster of 9 atoms using a procedure devised by Hirsch[17]. The data for the temperature dependence of the correlation funtions are shown in figures 12 and 13. For the lowest temperature one can reach, the local moment L_0 is about 70

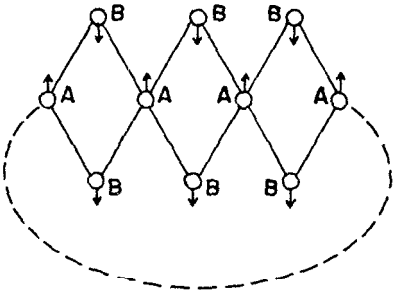

Fig. 11 - Cluster of 9 sitea with periodic boundary conditions used to simulate an almost-one-dimensional bipartite lattice. The figure shows the ground state spin configuration with the sublattices A and B ferromagnetically ordered but in opposite directions. Each unit cell has net spin 1/2 in agreement with Ref.13.

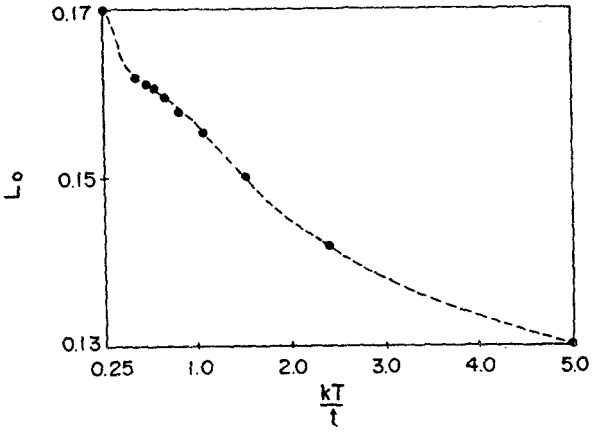

Fig. 12 - Temperature dependence of the local moment for the cluster of Fig.11 (U = 2). The line is a guide to the eyes.

% of the value for a completely localized spin. The type of magnetic arrangement is evidenced by the correlation functions L_1, L_2 and L_3. As $L_1 < 0, L_2 > 0$ and $L_3 < 0$ for all temperatures investigated, we conclude that in the ground state each sublattice is ferromagnetically ordered but in opposite directions, such that

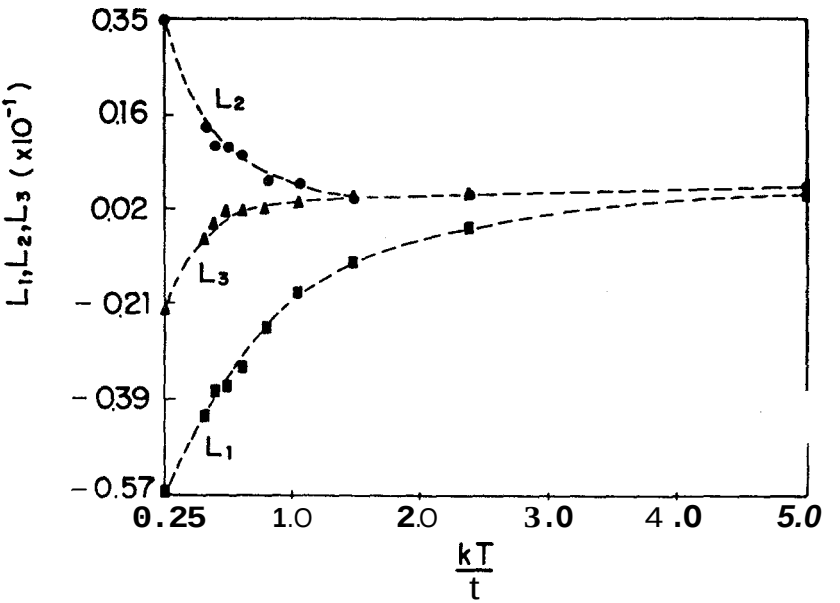

Fig. 13 - Temperature dependence of the first (L_1)- second (L_2) - and third (L_3) - neighbor correlation functions for the cluster of Fig.11 $(U = 2)$. The lines are guides to the eyes.

the total spin of the cluster is $S = 3/2$ in agreement with Lieb's theorem (see Fig.11). As the spin per unit cell is unsaturated, the predicted ferrornagnetic state is in fact a USF phase as pointed out by Lieb.

4. Conclusions

In this work we have investigated the occurrence of ferromgnetism in itinerant electron systems described by the one-band Hubbard model. Two different systems have been studied. In the first one we have exactly diagonalized clusters of 4 to 6 sites by increasing the primitive tetrahedral cell of an f.c.c. lattice such as to maximize the number of bonds. Several ground state properties have been calculated and a magnetic phase diagram was reported. Saturated ferromagnetisrn, unsaturated ferromagnetism and paramgnetism are found under certain values of the parameters characterizing the systems. Our findings compare well with those obtained using exact diagonalization[14] and approximate bulk techniques[15,16]. Relevant dicrepancies between the results derived for the cluster systems and those

obtained in the thermodynamic limit of the f.c.c. lattice[15,16] are also pointed out. In the second system we verify a recent theoreni by Lieb[13] in which unsaturated ferromagnetism is predicted for *half-filled* bipartite lattices with distinct numbers of sublattice sites in the unit cell. We take the simplest almost-one-dimensional periodic lattice and indeed verif that the calculated ground state spin is in agreement with the theorem. The calculations are made for clusters of 6 and 9 sites using exact diagonaiization and quantum Monte Carlo simulation.

In conclusion, our results provide evidence that itinerant-electron ferromagnetism occur in the *one-band* Hubbard model, even in the *half-filled* band case for special bipartite lattices.

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Resumo

Neste trabalho apresentamos resultados da diagonalização exata do modelo de Hubbard em aglomerados de **4,5** e 6 sítios, crescendo a célula unitária tetraedrica e obedecendo às simetrias da rede f.c.c. Calculamos diversas propriedades do estado fundamental tais como, o espectro de energias, o spin total dos aglomerados e funções de correlação de spin, as quais permitem a obtenção de um diagrama de fases magnéticas. Expomos também sobre resultados da diagonalização exata e simulação numérica de um sistema quase unidimensional, o qual acreditamos ser a rede periódica mais simples a exibir ferromagnetismo em uma banda semi-cheia, de acordo com um recente teorema demonstrado por Lieb.

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