Chapter 7

Single-Band Hubbard Model

7.1 Introduction

The single-band Hubbard model is believed to describe well the low-energy physics of high $T_c$ superconductors. Our calculations presented in Chapter 6 bring further evidence in favor of this statement. We started with a more realistic model which includes, aside from the correlated Cu $d_{x^2−y^2}$ orbitals, also the in-plane $p_x$ and $p_y$ oxygen orbitals and showed that the physics can be well approximated by a single band $t − t′ − U$ Hubbard model. The next-nearest-neighbor hopping integral $t'$ has an essential role in explaining the electron-hole asymmetry observed in the phase diagram, susceptibility functions and one-electron spectral functions.

Since the discovery of high $T_c$ superconductors the Hubbard model and the closely related $t−J$ model were under intense investigation. Many approximation schemes both analytical and numerical were used, but reliable results are difficult to obtain because the approximations involved are uncontrollable. The Dynamical Cluster Approximation technique, which considers a periodic cluster of size $L_c \times L_c$ embedded self-consistently in an effective-medium and takes $(\xi/L_c)^2$ as the small parameter which controls the calculation, we believe to be very promising in this respect. Here $\xi$ represents the antiferromagnetic correlation length which, based on neutron scattering experiments data [1], it is believed to be short-ranged in cuprates. Even the small $2 \times 2$ cluster seems to be large enough to capture the basic physics of the cuprates. The phase diagram calculated by M. Jarrell et al. [2] and shown in Fig. 6.14 with the dashed line exhibits antiferromagnetic, pseudogap and $d$-wave superconductivity regions, resembling the general phase diagram of cuprates (see Fig. 1.3). The DCA provides another important result, also in agreement with the recent experimental data, which shows that the superconductivity mechanism in cuprates is driven by the reduction of the kinetic energy below the critical temperature. Early on, analyzing the photoemission spectra, Norman et al. [3] pointed out that the superconductivity in cuprates could be a result of a kinetic energy gain rather than a potential one characteristic for normal BCS superconductors. This was confirmed by recent optical experiments [4] which show a transfer of the conductivity spectral weight from large to small frequency below $T_c$. Using DCA, Th. Maier et al. [5] calculated the kinetic and the potential energies of the normal and superconducting states below $T_c$. For the superconducting state the DCA code is modified to allow electron pairing, i.e. a non-zero value
for the off-diagonal elements of the Green’s function, Eq. 1.16, is permitted. The normal state is calculated imposing all the group symmetries on the Green’s function. The results are shown in Fig. 7.1. In the superconducting state, unlike the potential energy, the kinetic energy strongly decreases with decreasing the temperature. The kinetic energy is also lower than the normal state one, showing that that the superconductivity is a kinetic energy driven mechanism.

Considering a larger cluster is the next natural step in DCA calculation. The computational time required for the calculation scales as $N_c^3$, but the rapid increase in the performance of supercomputers around the world makes us very optimistic that in the very next future we will be able to perform systematic calculations on 16 site and even larger clusters. In this chapter we are going to present the results obtain for $t - U$ and $t - t' - U$ Hubbard models when a $N_c = 8$ cluster is considered. Compared to the $N_c = 4$ cluster case, most of the qualitative physics remains the same but also some important differences are noticed, and also new physics, as phase separation in the electron-doped $t - t' - U$ Hubbard model, appears too.

Looking carefully at the data available so far it can be noticed that the $N_c = 4$ case is rather special. M. Jarrell et al. [6] calculated the Neél temperature at zero doping

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**Figure 7.1:** Kinetic (top) and potential (bottom) energies of the normal (NS) and superconducting state (SC) as a function of temperature for low doping ($\delta = 0.05$, left) and high doping ($\delta = 0.20$, right). The vertical dotted lines represent the value of $T_c$. Pairing is mediated by a reduction of the kinetic energy. Calculated by Th. Maier et al. [5] with $t = 0.25 \text{ eV}, U = 2 \text{ eV}$.
for different cluster sizes. We show their results in Fig. 7.2. From the inset it can be seen that, except for the $N_c = 4$ case, the antiferromagnetic temperature is decreasing slowly with the number of sites in the cluster. Because the mean-field character of the DCA calculation results in a finite temperature transition when the correlation length exceeds the cluster size, this indicates that the spin-correlation length increases rapidly with decreasing the temperature $^*$. However the Neél temperature for $N_c = 4$ cluster does

$^*$For example, if the the spin-correlation length is assumed to vary as $\xi = e^{A/T}$ where $A$ is a constant of the order of the exchange coupling, we should expect a logarithmic decrease of $T_N$ with increasing $N_c$ [6].
not fit the general behavior, being much smaller. The critical exponent $\gamma$ is also very large ($\gamma = 1.29$ compared to $\gamma = 1.07$ corresponding to the $N_c = 8$ case) indicating strong fluctuations. Presently, this anomalous behavior of the $2 \times 2$ cluster is not completely understood. We believe it is related with the fact that the periodic boundary conditions imposed by DCA on the cluster introduce some artificial effects. It was shown that these errors become quickly negligible when the cluster size is increased, the DCA converging as $O(1/L_c^2)$ [7]. The convergence is much faster than it would be if a cluster with open boundary conditions embedded in a host is considered, the later approach being called Cellular Dynamical Mean Field Theory [8, 9] and converging as $O(1/L_c)$. However the $2 \times 2$ cluster with periodic boundary conditions has a fundamentally different topology from larger clusters. The coordination number for the $N_c = 4$ cluster is two while for the larger clusters it is four. This can be seen from Fig 7.3-a where the $N_c = 4$ cluster with periodic boundary conditions is shown. It is known that a small coordination number (smaller than four) favors the “singlet liquid” Resonance Valence Bond (RVB) [10] kind of solution to the antiferromagnetic Neél one. Therefore this could be the main reason for such a small $T_N$ obtained in the four site cluster calculation. In fact the exact diagonalization of the Heisenberg model on a $2 \times 2$ cluster with periodic boundary conditions shows that for this cluster the ground state is exactly the nearest-neighbor RVB state and this is a very stable solution, the excitation gap being much larger than the one corresponding to other clusters (the gap is equal to $2J$ which is 3.5 times larger than the $4 \times 4$ cluster excitation gap) [11]. Therefore it is reasonable to assume that even when the cluster is coupled to the effective host the special topology introduced by the periodic boundary conditions on the $2 \times 2$ cluster will stabilize the RVB configurations in detriment to the antiferromagnetic Neél ones, resulting in a much smaller $T_N$.

Based on the fact that $T_N$ obtained for the $N_c = 8$ cluster fits well the curve shown in Fig. 7.2 which describes the general behavior of the antiferromagnetic temperature versus the cluster size, we believe that the eight site cluster calculations is more realistic than the corresponding four site cluster calculations. However one still has to be careful, because we expect the next-nearest-neighbor correlations to be significantly influenced

![Figure 7.3: a) $N_c = 4$ cluster. b) $N_c = 8$ cluster.](image)
Figure 7.4: \( t - t' - U \) Hubbard model with \( t = 0.45 \text{ eV}, t'/t = -0.3 \) and \( U = 3.6 \text{ eV} \). a) Charge susceptibility versus temperature at 5% electron doping. b) The hole density versus chemical potential. In the shaded region, for a particular \( \mu \) there are many solutions, each of them corresponding to a different number of holes.

by the cluster topology now. As a result of imposing the periodic boundary conditions, the next-nearest-neighbor coordination number is two, as can be seen from Fig 7.3-b. In order to estimate the errors due to the cluster topology, comparison to larger clusters should be done. Some preliminary \( N_c = 16 \) results show that the \( N_c = 8 \) and \( N_c = 16 \) physics is pretty close (even though some quantitative differences which have to be due to the topology of the eight site cluster, like the too small pseudogap temperature, are observed). Further investigation in this direction is required.

Nevertheless most of the physics is common for \( N_c = 4, N_c = 8 \) and (as much as we know so far) \( N_c = 16 \) clusters. Therefore we believe that all the common features are genuine characteristics of the single-band Hubbard models.

### 7.2 Phase Separation in the Electron Doped Regime

The electron doped cuprates are described by a \( t - t' - U \) Hubbard model, with a positive nearest-neighbor hopping integral, \( t' \), in the hole representation. The \( N_c = 4 \) charge susceptibility in the underdoped region (see Fig. 6.17) increases strongly with decreasing temperature below \( T^* \). When the eight site cluster is considered this effect becomes dramatic developing into a real divergence of the charge susceptibility. This can be seen in Fig. 7.4-a where the charge susceptibility versus temperature is shown for the 5% electron doped case. The divergence occurs very close to \( T^* \), i.e. close to the same temperature
where the downturn in the spin susceptibility is observed. However, this is an accident specific only to the eight site cluster which, for reasons related to the cluster topology, provides a too small $T^*$. For the $N_c = 16$ cluster, the pseudogap temperature is larger and therefore larger than the temperature where the charge susceptibility diverges (which we find is not significantly influenced by the cluster size).

The charge susceptibility reflects the modification in the hole number when the chemical potential is slightly changed

\[ \chi_{\text{charge}} = \frac{\delta n}{\delta \mu} \]  

(7.1)

Therefore the divergence of $\chi_{\text{charge}}$ indicates an instability in the hole density and suggests that the system suffers a first order transition to an inhomogeneous phase where regions with different hole densities are spatially separated.

The phase transition is characterized by the dependence of the hole number on the chemical potential. The instability in the number of holes makes the calculations which preserve the doping and adjust the chemical potential at every iteration very difficult. Usually this is the way in which our computations are done. But we can also run calculations which keep the chemical potential fixed. We noticed that, depending on the initial “guess” of self-energy, for a fixed chemical potential the DCA can converge to different solutions characterized by different hole density. This is shown in Fig. 7.4-b. The solutions shown with circles (solid line) are obtained starting from a chemical potential which corresponds to zero doing, where the divergence in the charge susceptibility is not present and where only one solution exists. The next calculation is done for a slightly smaller $\mu$ and the present calculated self-energy is taken as the initial “guess”. The same procedure is repeated in the subsequent calculations. When the chemical potential corresponds to about 8% doping the divergence in the susceptibility disappears and, again, there is only one solution. Let’s call this solution the small doped solution. On the other hand if we start with a $\mu$ corresponding to 8% doping and apply the same procedure, but with the difference that now at every subsequent calculation we increase the chemical potential, the result will be the one shown with squares (dashed line). We call this solution the large doped one. All the calculations described above are done at a temperature smaller than the susceptibility divergence temperature corresponding to 5% electron doping. The $(n, \mu)$ characteristic has a hysteresis shape showing explicitly that the transition is first order. For the temperature shown in the figure, the doping range where the system is instable towards phase separation is between a very small doping (0.5%) and about 8% doping. Presumably the hysteresis range increases at lower temperatures. We can conclude that the system likes to separate in two regions, a very lightly doped one and a about 8% doped one. The situation is similar to the familiar gas-liquid first order phase transition, the pressure and the volume being replaced by the chemical potential and respectively by the number of holes.

The exact diagonalization of the $t - t' - J$ model with a positive $t'$ (which corresponds to electron doping) shows that two holes on a small cluster like to stay in the vicinity of each other, suggesting the possibility of phase separation [12, 13]. This is not true for a negative or zero next-nearest-neighbor hopping integral when the holes prefer to stay at a large distance from each other. However the cluster size is too small to prove a real phase separation, but at least the exact diagonalization shows that our results are not
7.3 Phase Diagram

In this section we discuss the $t-U$ and $t-t'-U$ Hubbard model phase diagrams calculated with DCA on a $N_c = 8$ cluster. They are shown in Fig. 7.5. The electron-hole asymmetric $t-t'-U$ model is plotted with solid line and the symmetric $t-U$ model with dashed line.

Compared to the $N_c = 4$ phase diagram (see Fig. 6.14), the $N_c = 8$ one shows some important differences. The most significant one is the large Neél temperature and the large critical doping where the antiferromagnetism disappears (the antiferromagnetism persists up to 20% doping for the $t-U$ Hubbard model).

Normally, in order to account for correlations larger than the cluster size antiferromagnetic, below $T_N$ we should work with a broken symmetry solution, i.e. to couple the cluster with an antiferromagnetic host whose properties follows to be determined self-consistently. This work requires some modification to the present DCA code and has not been done yet. Instead, even below $T_N$ we keep working with a paramagnetic solution which implies that the cluster is coupled to a medium characterized by spin rotational invariant properties. In this way we suppress (artificially) the antiferromagnetic correlations longer than the cluster size. Therefore we should consider the physics obtained below $T_N$ as a characteristic of the Hubbard model with suppressed long-range antiferromagnetic correlations. It is possible that the same features remain when the longer-range correlations are included.

Figure 7.5: $t-t'-U$ Hubbard model (solid line) and $t-U$ Hubbard model (dashed line) phase diagrams calculated for a $N_c = 8$ cluster. $t = -0.45$ eV, $t'/t = -0.3$, $U = 3.6V$ quite unexpected.
correlations are allowed, but this has to be checked.

The next-nearest-neighbor hopping integral has the same influence on the antiferromagnetic properties as we determined for the $N_c = 4$ calculations. In the undoped regime $T_N$ is decreased by $t'$. The critical doping where the antiferromagnetism disappears is reduced (increased) in the hole (electron) doped regime.

Below $T_N$ we find pseudogap and $d$-wave superconductivity, similar to experimental data. The pseudogap temperature $T^*$, which is determined from the downturn in the spin susceptibility is much lower than the antiferromagnetic temperature. Preliminary calculations show that it increases again for the $N_c = 16$ cluster (but it still remains lower than the corresponding $T_N$). This suggests that the next-nearest-neighbor correlations (which presumably are the most affected by the periodic boundary conditions imposed on the $N_c = 8$ cluster) have an important contribution in this matter and are suppressing the pseudogap in the $N_c = 8$ case. The effect of $t'$ on the spin susceptibility is the same as for the $N_c = 4$ case. The $t'$ corresponding to hole doped regime makes the susceptibility increase and the downturn at $T^*$ to sharpen with increasing the doping. The opposite effect is seen for the electron doped case.

For the $N_c = 4$ cluster we found that the superconductivity persists up to a very small doping (less than 1%) with a maximum $T_c$ around 5% doping. The $d$-wave superconductivity region looks more realistic for the $N_c = 8$ cluster, for example the $t-U$ Hubbard model doping range is between 5% and 20% with a maximum $T_c$ around 15% doping. Preliminary calculations with a $N_c = 16$ cluster indicates that these features remain when the cluster size is increasing. Switching on $t'$ the superconductivity moves towards larger dopings in the hole doped regime. In the electron doped case the critical doping where the superconductivity disappears is reduced and the superconducting region shrinks. Similar to what we observed for the $N_c = 4$ case, $t'$ has no significant influence on the maximum value of the critical temperature, $T_c^{\text{max}}$.

As we discussed in Section 7.2, in the electron-doped regime $t'$ gives rise to phase separation when the doping is smaller than 8% – 9%. For the $N_c = 8$ cluster we find that the phase separation temperature $T_{ps}$ more or less coincides with the pseudogap temperature $T^*$. For the $N_c = 16$ cluster $T_{ps}$ remains the same but $T^*$ increases, thus the phase separation takes place below the pseudogap temperature.

### 7.4 Density of States and Pseudogap

One of the great advantages of the DCA technique is the possibility to calculate the density of states and the momentum dependent spectral functions, thus making possible a direct comparison between the calculated spectra and the experimental photoemission ones. The $N_c = 4$ cluster calculation of $t - t' - U$ Hubbard model shows that the hole doped and the electron doped spectral functions are different. In the hole doped case the pseudogap is located around the $(0, \pi)$ and $(\pi, 0)$ points in the Brillouin Zone, in agreement with experimental data. On the other hand, in the electron doped case we did not detect any pseudogap features around these points. This seems to be in agreement with the experiment too, the photoemission showing in this case a pseudogap at $(\pi/2, \pi/2)$ and Fermi pockets at $(0, \pi)$ and $(\pi, 0)$ [14]. However, the small four site cluster implies a
Figure 7.6: Coarse-graining of Brillouin Zone in eight cells \((N_c = 8)\) around \(K = (0,0), (\pm \pi/2, \pm \pi/2), (0, \pi), (\pi, 0)\) and \((\pi, \pi)\).

Figure 7.7: \(t-t'-U\) Hubbard model DOS at 5% electron doping. \(t = -0.45\) eV, \(t'/t = -0.3\), \(U = 3.6V\)
too rough coarse-graining of the Brillouin Zone (see Fig. 6.13) and does not allow us to study the spectral function around \((\pi/2, \pi/2)\). But the \(N_c = 8\) cluster is large enough for this purpose, the coarse-grained Brillouin Zone containing a cell around \((\pi/2, \pi/2)\) (see Fig. 7.6).

The total density of states (thick solid line) and the momentum dependent spectral functions around \((\pi/2, \pi/2)\) (thin solid line) and around \((0, \pi)\) (dashed line) at 5\% electron doping is shown in Fig. 7.7. The temperature is below \(T^*\) and the pseudogap is clearly seen in the total DOS and in the momentum dependent spectra around \((\pi/2, \pi/2)\), thus in very good agreement with experiment.

However some important remarks should be made about the calculation of DOS in the electron underdoped regime. We found the pseudogap temperature, \(T^*\), to be equal to the phase separation temperature, \(T_{ps}\). In order to see a well developed pseudogap, spectra at temperatures well below \(T^*\) should be calculated. But this implies that we go into the instable region where the phase separation takes place and where for the same \(\mu\) a smaller doped and larger doped solutions exist (and of course any linear combination of them). The DOS presented in Fig. 7.7 corresponds to the large doped solution (analogue to the dashed line one shown in Fig. 7.4-b, the difference being that we are at a lower temperature). It would be interesting to see if the other solution (the small doped one) exhibits similar DOS features.

The eight site cluster DOS calculation for the hole doped regime has not been done yet.

### 7.5 Conclusions and Discussions

In this chapter we studied the properties of the single-band \(t - U\) Hubbard and \(t - t' - U\) Hubbard models with Dynamical Cluster Approximation using an eight site cluster. Increasing the number of cluster sites, the \(N_c = 8\) cluster is the first after the \(N_c = 4\) one which preserves the lattice symmetry.

Most of the \(N_c = 8\) physics is similar to the \(N_c = 4\) one, but also some major differences are present. The most important one is the large Ne\"el temperature and the large critical doping where the antiferromagnetism disappears. This causes almost all the interesting physics (pseudogap, superconductivity) to take place below \(T_N\). The large \(T_N\) is not a peculiarity of the \(N_c = 8\) cluster because similar large \(T_N\) are also observed when larger clusters are considered, but rather the \(N_c = 4\) cluster is special. We argue that this anomalous behavior of the \(2 \times 2\) cluster comes form the special topology which results when the periodic boundary conditions are imposed. As exact diagonalization shows the periodic boundary conditions on a four site cluster stabilize strongly the singlet liquid (nearest-neighbor RVB) configurations, and we believe this is the reason for the suppression of the antiferromagnetism.

Normally, the calculation below \(T_N\) should be done by coupling the cluster to an antiferromagnetic host. This work has not been done yet. Instead we keep working below \(T_N\) with the same paramagnetic code (rigorously suitable only above \(T_N\)) which constrains the host to be symmetric. This will destroy artificially the longer than the cluster size antiferromagnetic correlations. Therefore the validity of our conclusions is restricted to
systems with short-range antiferromagnetic correlations. The conclusions might still be true when longer than the cluster size correlations are allowed, but this has to be checked.

Below $T_N$, in the underdoped region, looking at the spin susceptibility and at the density of states we find the characteristics of the pseudogap physics. The $d$-wave superconductivity present at very small doping in the $N_c = 4$ cluster calculation is suppressed now. The doping range of superconductivity is more realistic, being between 5% and 20% for the $t-U$ model. The next-nearest-neighbor hopping integral, $t'$, influences the physics in the same way we found for the $N_c = 4$ case. In the hole doped regime it increases the critical doping where the superconductivity disappears and it has an opposite effect for the electron doped regime. Opposite to that, $t'$ enhances the antiferromagnetism in the electron doped case and suppresses it in the hole doped case.

For the $N_c = 4$ cluster, in the small electron doped region, the next-nearest-neighbor hopping results in a strong increase of the charge susceptibility below $T^*$. For the $N_c = 8$ cluster, $t'$ results in more dramatic effect, the charge susceptibility diverging at a temperature close to $T^*$. The same effect is also noticed for the $N_c = 16$ cluster, but here $T^*$ is larger than the phase separation temperature, $T_{ps}$. The divergence of charge susceptibility indicates a first order transition to a phase separated state. We find that below $T_{ps}$, for a fixed chemical potential, depending on the initial guess of the self-energy, the DCA converges to two solutions, a small doped and a large doped one. Thus the particle number-chemical potential characteristic has a hysteresis shape, and studying it we conclude that the system is instable towards separation in two regions with different doping, a very lightly doped one, ($\approx 0.5\%$) and another one with a larger doping ($\approx 8\%$).

Form the $N_c = 4$ calculation we concluded that $t'$ is responsible for the electron-hole asymmetry seen in the ARPES spectra. However, because of the coarse-graining of the Brillouin Zone in only four cells, we could not study the spectral function near $(\pi/2, \pi/2)$ where the pseudogap was experimentally found in electron-doped cuprates. The $N_c = 8$ cluster makes this possible, and we find a pseudogap at $(\pi/2, \pi/2)$ indeed. However we should mention that the spectra were calculated below $T_{ps}$, thus in the region instable towards phase separation, and our DOS corresponds to the larger doped solution. If the same features are present for the other solution remains to be checked.

The $N_c = 8$ Dynamical Cluster Approximation study of the Hubbard model brings new results but also reveals some problems with the technique when it is applied to very small clusters where the imposed periodic boundary conditions have a significant effect. However the exact diagonalization results shows that for clusters larger than or equal to $4 \times 4$ these effects become negligible, and the present computing resources already allows us to study the $4 \times 4$ cluster. But even the small $N_c = 4$ and $N_c = 8$ clusters results are valuable, but one has to be cautious with the physical interpretation. Comparing the $N_c = 4$, $N_c = 8$ and some preliminary $N_c = 16$ calculations we noticed a similar physics. They all exhibits antiferromagnetism, pseudogap and $d$-wave superconductivity. The difference consists only in magnitude of these phenomena. We believe that through an understanding of the periodic boundary conditions influence on the DCA results, we can find a way to control these properties. For example, the $N_c = 4$ cluster enhances the next-nearest-neighbor RVB configurations and as a result the antiferromagnetism is reduced and the pseudogap and the superconductivity are enhanced. Allowing long-range antiferromagnetic correlations we can determine if the superconductivity and the
pseudogap are enhanced, suppressed or whether they disappear completely. Based on the \( N_c = 4 \) results we believe that one of the last two options is true. If so, in order to explain the experimentally determined properties of the cuprates we can argue that some other interaction which stabilize the singlet formation in detriment to long-range antiferromagnetism should be considered. A possible and reasonable candidate for this purpose could be the electron-phonon interaction, which we found in Chapter 4 to favor the nearest-neighbor singlet formation when the Coulomb repulsion is large. Besides we have the advantage that phonons can be introduced easily in DCA, so that the study of the above proposed scenario is perfectly possible. That would be a continuation of the present work, making also the natural connection between the first and the last part of this thesis.
References


