1 Introduction.

The Hubbard model has been the simplest starting point in the study of strongly correlated systems\cite{1, 2, 3}. Almost all methods known to condensed matter theoreticians have been applied to its analysis.

Much progress has been achieved in the 1D version of the model, starting from the exact description of the ground state wavefunction\cite{4}. Its behavior as function of the dimensionless coupling constant, $U/t$, and band filling, $n$, is representative of all 1D Luttinger liquids. These are characterized by a vanishing quasiparticle pole at the Fermi surface, a gapless spin and charge excitation spectrum, and the separation of spin and charge.

The situation in other dimensions is much more unclear. There is ample evidence that the model, at half filling and in a bipartite lattice, is an insulator with long range antiferromagnetic order. Some progress has been made in the study of the model in infinite dimensions\cite{5} and at half filling, where a metal insulator transition can be proved to exist in any lattice. The limit of a low electron density starts to yield to a variety of techniques\cite{6}. The established consensus is that the system behaves like a normal Fermi liquid, although the 2D case is still open to controversy. The rest of the phase diagram, especially in the interesting case of 2D near half filling, remains to be understood satisfactorily.

Among the many methods used in the analysis of the model, it is somewhat surprising the low attention given to standard mean field schemes, like the Hartree Fock approximation, and extensions thereof. Most of our understanding of conventional materials has been obtained from these methods.
On the other hand, the electron-electron interaction is, in general, comparable to the other terms in the Hamiltonian. The success of the Hartree-Fock methods is due to the fact that most effects of the electron-electron interaction can be accounted for by means of an appropriately chosen effective potential. The validity of Landau’s description of quasiparticles in a Fermi liquid depends on this assumption. A rather comprehensive description of the properties of simple metals can be obtained from the Hartree-Fock and Random Phase approximations.

Despite the successes reported above, mean field schemes are traditionally considered inadequate for the study of strongly correlated systems. To our knowledge, two main reasons are argued to support this conclusion:

- The Hartree-Fock method fails to describe, even qualitatively, the physics of the “canonical” model of strongly correlated electrons, the Anderson impurity. No hint of the Kondo effect can be deduced from such an analysis.
- The other well understood unconventional strongly correlated system is the 1D Luttinger liquid. Again, a naive application of standard mean field techniques fails to capture the main physical properties, described before.

It is worth to study in detail the advantages and shortcomings of the Hartree Fock approximation in view of these two apparent catastrophic failures:

- HF and the Anderson model. The Anderson model is an isolated “Hubbard atom” interacting with a Fermi gas. Its behavior shows different regimes, characterized by the energy scales of the problem:

  Below energies of order $U$, double occupancy of the site becomes irrelevant, and the only degree of freedom left is the spin of the impurity.

  There is a lower scale defined by the hopping of the electrons to and from the impurity, $\Gamma$. At energies where double occupancy is frozen out, this term generates an effective antiferromagnetic coupling, $J \sim \Gamma^2/U$.

  Finally, there is still a lower scale, which gives the binding energy of the singlet formed by this antiferromagnetic coupling, $T_K \sim J \exp[-N(\epsilon_F)J]$.

  The system shows a crossover between a high temperature regime, where the impurity spin fluctuates, weakly coupled to the rest of the $N$ electrons, and a low $T$ behavior, characterized by an almost frozen singlet, decoupled from the remaining $N - 1$ electrons.

  The failure of the HF approximation to capture the low $T$ physics can be traced back to the existence of this crossover. A single effective potential will never describe two quite different regimes. The potential adjusts itself to optimize the description of most of the effects which give shape to the wavefunction. The processes above $T_K$ are reasonably described by the H-F method, from the suppression of double occupancy down to the existence of an antiferromagnetic interaction.

- The 1D Luttinger liquid. Here, the situation is different, as these systems do not exhibit any kind of crossover. Standard application of HF leads to a spin density wave (for the 1D Hubbard, for example), with a gap in the spectrum, for any filling. The existence of this gap, and the breaking of trans-
lational invariance by the SDW are taken as serious failures of the method. However, it can be shown that these features are not such unsurmountable problems:

The 1D Hubbard model does not exhibit a true gap, even within HF, except at half filling. In order to compute the energy required to add an extra electron, it is best to compare the total energies of wavefunctions with different number of electrons. These energies show no discontinuity, except at half filling. The extra electrons do not fill the lowest state above the gap in the initial solution, but give rise to a rearrangement of the SDW and of the wavefunction. Moreover, this rearrangement of the entire many body state leads to $Z = | < \Psi_N | c_k^+ | \Psi_{N-1} > |^2 \to 0$. Thus, the disappearance of the quasiparticle pole can also be described within HF.

The breaking of translational symmetry is required in order to account for the strong shake up effects induced by extra electrons, which lead to the vanishing of coherent quasiparticles. The random phase approximation suffices to restore this symmetry, giving a zero mode associated with the motion of the SDW. The RPA also gives a difference between the velocities of the low energy spin and charge collective excitations, which are missing at the HF level.

Thus, a judicious application of the HF and RPA methods leads to the most relevant features of the 1D Luttinger liquid: absence of the quasiparticle pole, gapless excitations, and separation of spin and charge.

In the following, we will make use of these considerations to explore the phase diagram of the 2D Hubbard model in a square lattice.

2 Mean field solutions.

The Hartree Fock scheme can be implemented with a variety of constraints. Usually, the equations are solved in Fourier space, assuming that some kind of spin and charge density wave exists. The possible wavevectors for these distortions are given by the size of the unit cell considered. The amplitudes of these possible waves can be seen as variational parameters to be optimized.

This procedure suffices to give a reasonable description of a conventional system in most cases. For the Hubbard model, and at half filling, we find as the best solution an antiferromagnetic SDW, with the spins in the two sublattices pointing in opposite directions. A normal, paramagnetic metal is also described by a Slater determinant made up of plane waves, which is a HF solution of the Hubbard model with a sufficiently dilute concentration of electrons.

Near half filling, however, many solutions appear which cannot be described in such a simple way. Thus, we are forced to solve the selfconsistent HF equations in finite clusters, without imposing any constraints on the shape of the effective potential. Open and periodic boundary conditions are used. The most striking result obtained is that many different selfconsistent solutions (local minima) are found. As the solution is found by an iterative procedure, the final shape depends on the initial guess for the wavefunction.
This fact is presented in fig. (1), where two typical textures are shown (for a more detailed description of the solutions, see [7]).

Figure 1. HF antiferromagnetic ground state at half filling (left), and spin and charge texture for 10% doping (right). The arrows denote the spins, and the circles stand for the deviation of the local charge from 1 (half filled band).

Clearly, these wavefunctions break translational symmetry, as in the 1D case mentioned in the introduction. The number of solutions greatly increases with the size of the system. Note that the cluster sizes are much larger than the typical correlation length in the AF phase, $\sim t/\Delta$ lattice units, where $\Delta$ is the AF gap. The energies of these textures fluctuate strongly with cluster size, filling and value of $U/t$. Thus, it is impossible, in practical terms, to define the best HF solution of a cluster of moderate size, near half filling.

This richness of textures difficults the study of the model, but also points out to important physical features of the Hubbard model. The large number of metastable minima of the HF energy suggest the existence of glassy behavior. The underlying frustration is due to the competition between the repulsion and the kinetic energy, complicated further by anisotropy effects, which are greatly enhanced near half filling.

The solutions can be classified, in broad terms, into magnetic polarons, domain walls and vortices. Domain walls are a direct consequence of the nesting near half filling $\delta$, and are most stable at low doping and small values of $U/t$. Magnetic polarons are localized textures which resemble small ferromagnetic bubbles in an AF background. They dominate for large values of $U/t$. There is a smooth crossover from extended polarons to circular
domain walls, as function of doping and $U/t$. Finally, vortices arise because of the additional $U(1)$ symmetry provided by the phase of the wavefunction. They tend to appear at intermediate values of $U/t$. Periodic arrays of these solutions are found for sufficiently large cluster sizes. There is a wide variety of other, less regular, textures in large clusters. Among them, it is worth mentioning that, for certain dopings, holes tend to form localized pairs with p-wave symmetry. These pairs have a finite binding energy. These solutions suggest the possibility of superconductivity for a small region of parameter space.

3 Excitation spectrum. RPA.

We have computed the excitations within the Random Phase Approximation\cite{9}. This extension of the Hartree Fock method is crucial in order to obtain correctly the low energy spin waves. The initial HF excited states, however, are a reasonable guide for the charge excitations, which are not so strongly modified by the inclusion of the self consistency by the RPA.

Figure 2. Density of states for the two HF solutions shown in figure 1. The chemical potential for the doped case lies at $\omega = 0.95$.

The HF density of states is shown in fig. (2), for two characteristic situations: a) At half filling, the system is an insulator, with a gap in the charge excitation spectrum of order $U$. b) Near half filling, a number of localized states appear within the AF gap. The Fermi level remains at the edge of the relevant band. The level structure is by no means rigid, as the number of states within the gap is proportional to the number of holes. Note
that all these features are consistent with results obtained from the exact
diagonalization of finite clusters [10].

The states within the gap imply that, away from half filling, a continuum
of low energy charge excitations exists. This picture for the charge-charge
channel remains qualitatively unaltered when the RPA is fully implemented.
On the other hand, the spin waves can only be described within the RPA.
As function of doping, the total spectral strength in the spin wave band
decreases proportionally to the number of electrons or holes. The density of
low energy excitations, for a case near half filling, is shown in fig. (3).

We have also computed, because of its experimental relevance, the density
of excitations at the corner of the Brillouin zone, \((\pi, \pi)\). At half filling,
there is a large peak at zero energy, due to the AF ordering. This peak
is broadened, and shifts to higher energies, as the doping increases. There
is no significant structure in the charge spectrum. This difference in the
spectral weights throughout the Brillouin Zone between the charge and spin
excitations persists up to quite large doping levels \((\approx 50\%, \text{ for } U/t = 10)\).

Figure 3. Density of spin and charge excitations for the two HF solutions shown
in figure 1. Dotted lines give the spin and dashed lines the charge excitations.
Thick lines represent results for the doped cluster. The curves in the left side are
integrated densities of excitations, while those at the right are excitations at the
\((\pi, \pi)\) point of the Brillouin zone.

The fact that charge and spin excitations show different dispersion in
momentum space is an indication of spin-charge separation. As mentioned
in the introduction, the RPA suffices for a qualitative description of this
phenomenon in 1D. In our case, the existence of a 2D dispersion relation, instead of simple sound waves, allows for a richer variety of phenomena, which will be studied elsewhere.

4 Quasiparticle strengths.

The proliferation of HF solutions which break translation symmetry suggests the relevance of shake up effects, induced by the injection of electrons or holes. As mentioned in the preceding section, the HF energy levels do not shift rigidly as function of the electronic density. The textures rearrange themselves, so as to accommodate the electrons in newly formed localized levels. In turn, these levels modify the underlying continuum.

The importance of these shake up effects can be estimated, within the Hartree Fock approximation, by computing the matrix element: $Z = | \langle \Psi_0(N) | c_i | \Psi_0(N + 1) \rangle |^2$. The operator $c_i$ is taken to be the lowest occupied electronic level in $| \Psi_0(N + 1) \rangle$. This procedure, although unusual in applications of the HF method, is perfectly well defined as an approximation to the spectral strength of the quasiparticle pole. In normal metals, this scheme gives $Z = 1$. This is due to the fact that most of the missing spectral strength goes into plasmon satellites. The description of this structure requires us to go one step beyond the HF + RPA procedure used here. In the Hubbard model, the depletion of the quasiparticle pole comes from low energy, electron-hole pairs. Their shake-up is approximately described by the rearrangement of the electronic levels in the HF Slater determinant. Thus, we expect, at least, a qualitative description of this effect within our approximations.

The results that we find are discussed in detail elsewhere in this volume (see also [1]). The most relevant feature is that, near half filling, the splitting from the continuum of localized states upon doping, leads to a vanishing $Z$. This result can be viewed as an ”orthogonality catastrophe”, induced by the phase shifts generated by these localized states in the continuum levels. Understood in these terms, the nature of the physical regime that we find near half doping is very similar to the 1D Luttinger liquids.

5 Conclusions.

We have presented a comprehensive study of the two dimensional Hubbard model in a square lattice, using mean field techniques. We find three different regimes:

- The system is an antiferromagnetic insulator at half doping. The low energy excitations are spin waves.
- Very far from half doping, the model behaves as a conventional Fermi liquid. The low energy excitations are electron-hole pairs. The doping required to reach this regime depends on the value of $U/t$, but it is always present.
- Near half doping, we find a phase quite reminiscent of the 1D Luttinger liquids. The system has no gap. At low energies, spin and charge excitations
coexist, although with different dispersion relations. There are strong shake-up effects upon the injection of electrons and holes, which lead to a vanishing quasiparticle pole.

In addition, our scheme also gives a ferromagnetic phase\cite{12}, for large values of $U/t$, and very close to half doping. This phase remains to be fully characterized.

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