Momentum dependence of the spin and charge excitations in the two dimensional Hubbard model

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The low energy spin and charge excitations in the 2D Hubbard model near half filling are analyzed. The RPA spectra derived from inhomogeneous mean field textures are analyzed. Spin excitations show a commensurate peak at half filling, incommensurate peaks near half filling, and a broad background typical of a dilute Fermi liquid away from half filling. Charge excitations, near half filling, are localized near (0,0), and they occupy a small portion of the Brillouin Zone, in a way consistent with the existence of a small density of carriers, and a small Fermi surface. At higher hole densities, they fill the entire BZ, and can be understood in terms of a conventional Fermi liquid picture. The results are consistent with the observed features of the high-Tc superconductors.

Despite its simplicity, the Hubbard model in two dimensions is poorly understood [1], although it is widely considered that it is a good description of the low energy physics of high-Tc superconductors [2].

Among other possibilities, it has been conjectured that, near half filling, it may show non trivial (marginal) behavior, without coherent quasiparticles [3], or that it is a strongly correlated d-wave superconductor [4]. One of the main stumbling blocks encountered in the study of this model is the absence of a scheme general enough to describe such widely different possibilities. Numerical calculations have been inconclusive with respect to the low energy behavior in the lightly doped, strongly coupled regime [5].

In the present work, we show that a global picture can be obtained from mean field calculations (unrestricted Hartree Fock) supplemented by the next leading order correction, given by the Random Phase Approximation. Note that such an approach does reproduce correctly the main features of the Hubbard model in the regimes where a consensus about its behavior has been reached:

i) It describes a Luttinger liquid in 1D.
ii) It gives an antiferromagnetic insulator at half filling in a bipartite lattice.
iii) It reproduces Fermi liquid behavior at low electron densities.
iv) It satisfies Nagaoka’s theorem for sufficiently low doping and large values of $U/t$.

It is commonly accepted that a mean field description suffices to understand regimes ii), iii) and iv). In all cases, the ground state wavefunction is well approximated by a Slater determinant (although, in order to obtain correctly the low energy excitations of an antiferromagnet, the RPA needs to be used).

What is not so widely appreciated is that, with some hindsight, the main features of a Luttinger liquid can also be inferred from such a mean field + RPA fluctuations approach. In fact, the spin and the charge RPA polarizabilities of a 1D gapless Fermi system differ by a sign in the denominator, ($\chi_{RPA} \sim \chi_0/(1 \pm U\chi_0)$). As, in 1D, the only excitations are associated with poles in $\chi$, this non trivial difference in sign shifts the pole in the spin-spin channel with respect to that in the charge-charge channel, leading to spin-charge separation. In addition, it can be shown that the injection of additional electrons leads to alterations in the self consistent Hartree Fock wavefunctions. These changes, in turn, renormalize the quasiparticle weight, which vanishes in 1D, and near half filling in 2D [6]. Thus, this approach correctly identifies the two characteristic features of a Luttinger liquid: the absence of a quasiparticle peak at low energies, and the separation of spin and charge [4].

We now study the spin and charge excitations of the 2D Hubbard model, within the RPA. To do so, we use as starting point, the self consistent solutions at finite dopings extensively discussed earlier [5]. The most characteristic feature of these solutions is that, except for half filling or for a very small number of particles, they correspond to inhomogeneous spin and charge textures. These wavefunctions, which break the translational symmetry of the Hubbard Hamiltonian, have always a lower energy than the homogeneous ones. The same spontaneous breaking of translational symmetry occurs when applying mean field techniques to 1D systems: it is the origin of the well
known SDW or CDW instabilities. This instability reflects the failure of standard perturbation theory around the unperturbed wavefunction.

In principle, translational symmetry can be restored by hybridizing equivalent textures, shifted by a given lattice vector. This procedure is equivalent to project the $\vec{k} = 0$ component of the initial wavefunction. It was shown in [9] that, in this way, an effective mass for the local textures (“spin polarons”) can be obtained, along with other non trivial features later confirmed by other numerical techniques, like the tendency of the defects to hop within a given sublattice only. Analogously, rotational symmetry can be retrieved by projecting the $S = 0$ component of the inhomogeneous wavefunction. Note that, for the half filled case, the translational and rotational symmetry breaking present in the Hartree Fock wavefunction reproduces the accepted features of the exact solution.

In the present work, however, we have not tried to restore translational symmetry. The RPA response functions, instead, are analyzed in Fourier space. We obtain an approximation to matrix elements of the type $\langle 0 | \hat{A}(\vec{k}) | n \rangle$, where $\hat{A} = \hat{S}, \hat{Q}$. It was shown in [9] the hybridization effects do not change significantly the main features of the wavefunctions, except for giving a finite hopping amplitude to the local defects. Thus, we expect the lack of translational invariance to be a higher order effect. Our calculations also depend on the choice of spin texture, for a given filling and value of $U/t$. As discussed in [10], the Hartree Fock equations admit a variety of nearly degenerate, inhomogeneous, self consistent solutions, and it is almost an impossible task to identify the optimal one. It is likely that, in addition, this richness of solutions is physically meaningful, being associated to the intrinsic frustration induced by the competition between commensurability and kinetic energy minimization. In the following, we use “spin polaron” solutions, which describe best the low energy states for intermediate to large values of $U/t$, and a wide range of dopings. These textures correspond to solutions in which holes are localized in a given site, in which the spin is flipped and reduced, with the remaining structure retaining its antiferromagnetic order. We have checked that the main features reported below are insensitive with respect to the type of texture being considered.

The analysis performed here was described in [10]. We calculate:

$$\chi(\omega) = [\mathcal{I} \pm U \chi_0(\omega)]^{-1} \chi_0(\omega)$$

(1)

where $\chi$ is written, in real space, as a $4N \times 4N$ matrix, for a system of size $N \times N$. The four components per site correspond to the three spin degrees of freedom (- sign in Eq. (1)) and the charge degree of freedom (+ sign in Eq. (1)).

Once $\chi$ has been obtained in real space, we define:

$$\chi(\vec{k}, \omega) = \sum_{i,j} e^{i\vec{k}(\vec{r}_i - \vec{r}_j)} \chi_{i,j}(\omega)$$

(2)

Our results allows us to identify four distinct regimes, as function of doping and coupling:

i) At half filling (one electron per site, $n=1$) the excitations correspond to those of a commensurate antiferromagnetic insulator. The only low energy excitations are the transverse spin modes, which are dominated by the commensurate peak at $(\pi, \pi)$ (fig 1). Charge modes have no weight at low energies, showing a gap of order $U$. This is an obvious case where the scheme used here approximates well the expected features of the exact solution. Note that, in this situation, the spin and charge excitations are clearly separated.

ii) Near half filling, the spin and charge excitations show very different, almost opposite, dependence on $\vec{k}$. The spin excitations move away from the $(\pi, \pi)$ position, giving rise to four incommensurate peaks at finite energies (figure 2a). We find, in addition, the remnants of the commensurate peak, which disappear at higher energies. Note that, for the range of $U/t$ values considered, these extra peaks cannot be ascribed to imperfect nesting. They are deformations of the AF background, more similar to the effects found in the lightly doped $t-J$ model. It is remarkable that these peaks survive the disorder in the textures used as starting point. The charge excitations (figure 2b), on the other hand, have peaks near $\vec{k} = (0, 0)$. They arise from the excitation of structureless states close to the Fermi energy. They resemble the excitations in a low density gas of electrons (or holes), also in agreement with the expected results in the $t-J$ model. As in the previous case, spin and charge excitations show almost non overlapping features in the $(\vec{k}, \omega)$ space. In addition, this regime corresponds to the vanishing of the quasiparticle pole, also within the unrestricted Hartree Fock approximation [9]. These features are also present in the 1D Luttinger liquid state, and are not expected in a conventional Fermi liquid, described in terms of Landau’s quasiparticles. The region where this behavior can be clearly identified is $n \geq 0.9$.

iii) Our results indicate the existence of a smooth crossover between the regime described above and a conventional Fermi liquid at low dopings. In this region, which covers most of filling fractions, the spectral strength of the low energy spin and charge excitations fall in different regions of the BZ (figures 3a and 3b). On the other hand, the eigenvectors of $\chi(\omega)$ show a mixture of spin and charge features. In general, this situation corresponds to the...
existence of a weak spin and charge texture in the initial Hartree-Fock configuration. In many cases, this texture is a well-defined spin density wave.

iv) In a sufficiently dilute system, our results are consistent with the existence of a normal Fermi liquid phase. The spin and charge background is uniform, and the local magnetization is zero everywhere. The RPA excitations show a 6 × 6 structure (figures 4a and 4b), which is due to finite lattice effects. This pattern is the same in the spin and charge channels, in agreement with the absence of spin-charge separation. We can establish the existence of this regime for filling fractions \( n \leq 0.5 \), for \( U/t = 5 \).

It is interesting to compare our results with the growing literature on the question of spin-charge separation in 2D. Almost all schemes concentrate on one electron properties, like the momentum distribution or the self energy.

Near half filling numerical and analytical calculations support the conclusion that a single hole in an antiferromagnetic background shows no quasiparticle pole [14]. Mean field results, along the approach discussed here, confirm this conclusion [14]. In the latter case, the analysis allows a rather straightforward description in terms of the orthogonality catastrophe [12]. This is consistent with the work reported here, as the low energy excitations do not exhibit an abrupt discontinuity from the half filled case, where the spin-charge separation is obvious.

Away from half filling existing approaches can be classified into numerical calculations [13-14], trial wavefunctions [13] and diagrammatic analysis [16]. Numerical evidence is difficult to interpret. Exact results for finite systems [14] have been used in support of spin-charge separation, based on the fact that the electronic momentum distribution resembles that of spinless electrons. Away from half filling, however, no evidence for spin-charge separation is found [13]. Alternatively, trial Luttinger-liquid-like wavefunctions [15], also support the existence of spin charge separation. Finally, self consistent diagrammatic schemes lead to self energies which do not show the expected Fermi liquid behavior [14]. Thus, there exists a consensus that, near half filling, the Hubbard model does not behave like a conventional Fermi liquid.

Our results corroborate the evidence discussed above. Moreover, they present a qualitative picture of the low energy spin and charge excitations, which clarifies the origin of the separation between the spin and the charge degrees of freedom. It should facilitate direct comparison with more phenomenological approaches based on the existence of strong short range antiferromagnetic correlations [7], which are being used to explain d-wave superconductivity in the high-T\(_c\) superconductors. The basic ingredient of these schemes is the existence of local moments aligned antiferromagnetically. That is indeed a feature present in our results.

Finally, it is worth mentioning that our results agree well with the measured magnetic properties of the high-T\(_c\) cuprates [13]. It would be interesting to check whether our predictions for the charge excitations can also be observed.

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Figure 1. Transverse spin excitations of the Hubbard model in a square lattice (12 × 12 sites) for $U/t = 10$, $n = 1$ (half filling) and $\omega = 0.1t$. $k_x$ and $k_y$ are plotted in units of $\pi/a$, where $a$ is the lattice constant.

Figure 2a. Charge excitations, calculated for $U/t = 10$, $n = 0.9$ and $\omega = 0.1$. Other parameters as in fig. 1. Figure 2b. Spin excitations.

Figure 3a. Charge excitations, calculated for $U/t = 10$, $n = 0.5$ and $\omega = 0.1$. Other parameters as in fig. 1. Figure 3b. Spin excitations.

Figure 4a. Charge excitations, calculated for $U/t = 5$, $n = 0.3$ and $\omega = 0.1$. Other parameters as in fig. 1. Figure 4b. Spin excitations.