Magnetic and Charge Correlations of the 2-dimensional $t - t' - U$ Hubbard model

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Abstract

Using a spin-rotation invariant six-slave boson representation, we study the square lattice Hubbard model with nearest-neighbor hopping $t$ and next-nearest neighbor hopping $t'$. We discuss the influence of $t'$ on the charge and magnetic properties. In the hole-doped domain, we find that a negative $t'$ strongly favors itinerant ferromagnetism over any incommensurate phase, especially in the strong coupling regime. For positive $t'$ magnetic fluctuations are suppressed. A tight connection between frustrated charge dynamics and large magnetic fluctuations is pointed out. A clear tendency towards striped charge ordering is found in the regime of large positive $t'$.

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I. INTRODUCTION

The spin rotation invariant slave boson representation is applied to the $t - t' - U$-model. This model is expected to be relevant to the physics of high-temperature superconductors, since it includes a reasonable description of their band structure. It is a good candidate for the description of itinerant ferromagnetism too. Both behaviors are expected to occur in different regions of the phase diagram. Indeed it can be thought of as consisting of three characteristic regions, depending on whether the magnetic fluctuations are strong or not, and whether they are ferromagnetic or anti-ferromagnetic. The size of these regions is tuned by $t'$. In the non-interacting limit the role of $t'$ is to shift the van Hove singularity that lies in the middle of the band for $t' = 0$ to the lower band edge for $t' = -t/2$ or to the upper band edge for $t' = t/2$. The extension of this physics to the weak coupling regime has been extensively studied by Lin and Hirsch [1], and Bénard et al. [2], and Lavagna and Stemman [3]. They found that, for large negative $t'$, the physics is dominated by strong ferromagnetic fluctuations in the low density domain, and by strong antiferromagnetic fluctuations in the vicinity of half-filling. Quantum Monte Carlo (QMC) simulations have been performed too. In particular Veilleux et al. [4] confirmed this behavior, and thus put it on a stronger basis. They also established that the static and uniform magnetic susceptibility goes over a maximum when the system is doped off half-filling. Recently Hlubina et al. [5] studied the same model at densities corresponding to the van Hove singularity, and found that the system is an itinerant ferromagnet for large negative $t'$, and an itinerant antiferromagnet for small negative $t'$. Unfortunately these techniques can only be applied in the weak to intermediate coupling regime, because of the minus sign problem for QMC simulations, and because the RPA is intrinsically a weak coupling approach. For strong coupling one usually resorts to variational methods [3,4], (for a recent discussion see [8]). In order to cover the entire parameter range it is tempting to apply the Kotliar and Ruckenstein slave boson approach [9]. It not only proved to yield ground state energies very close to the exact ones, but very realistic values for the structure factors too [10]. Until now little attention
has been paid to the charge structure factor. The aim of this brief report is two-fold. First we calculate the $q$-dependent magnetic susceptibility in order to determine in which domain of the phase diagram the antiferromagnetic, ferromagnetic and incommensurate fluctuations dominate, both in the intermediate and strong coupling regime. Second we calculate the charge structure factor. We then show that strong magnetic fluctuations are systematically accompanied with a clear reduction of the charge structure factor, i.e. by a frustration of the charge dynamics. In this model this happens for negative $t'$, in the hole doped region. For positive $t'$, the charge structure factor is enhanced and the magnetic fluctuations suppressed. We obtained this result using the spin-rotation invariant (SRI) slave boson representation of the Hubbard model [11,12], and the expression for the spin and charge dynamical susceptibilities we recently derived and applied to the Hubbard model [10]. We note that this representation has been recently revisited by Ziegler et al. [13]. Our expressions for the susceptibilities remain unchanged by their considerations.

II. FORMALISM

In this work we calculate the spin and charge dynamical susceptibilities of the two dimensional $t-t'-U$ model. The Hamiltonian reads:

$$H = - \sum_{i,j,\sigma} t_{i,j} c_{i\sigma}^+ c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

We consider the case where the hopping integral is $t_{i,j} = t$ for nearest neighbors, $t_{i,j} = t'$ for next-nearest neighbors and $t_{i,j} = 0$ otherwise. To this aim we apply the spin-rotation invariant (SRI) slave boson formulation of the Hubbard model [11,12] to the one-loop calculation of the susceptibilities that we applied to the Hubbard model. In this framework the dynamical spin susceptibility is given by

$$\chi_s(\vec{k}, \omega) = \frac{\chi_0(\vec{k}, \omega)}{1 + A_k \chi_0(\vec{k}, \omega) + A_1 \chi_1(\vec{k}, \omega) + A_2 \left[ \chi_1^2(\vec{k}, \omega) - \chi_0(\vec{k}, \omega) \chi_2(\vec{k}, \omega) \right]}$$

where
\begin{equation}
\chi_n(\vec{k},\omega) = - \sum_{\vec{p},\omega_n,\sigma} (t_{\vec{p}} + t_{\vec{p}+\vec{k}})^n G_{0\sigma}(\vec{p},i\omega_n) G_{0\sigma}(\vec{p}+\vec{k},\omega+i\omega_n) \quad (n = 0, 1, 2)
\end{equation}

In the low frequency regime Eq. (2) has an RPA form, to which it reduces in the weak coupling limit. It nevertheless differs from it in two important respects. First the effective interaction \( A_{\vec{k}} \) does not grow indefinitely as \( U \) grows, but saturates at a fraction of the average kinetic energy in the strong coupling regime. Second it is \( k \)-dependent. Therefore if an magnetic instability of the paramagnetic phase at a given density develops towards an incommensurate phase, characterized by a wave vector \( \vec{q} \), this wave vector will be different from the wave vector \( \vec{p} \) at which \( \chi_0(\vec{p},0) \) reaches its maximum. Thus at a given density, the wave-vector \( \vec{q} \) characterizing the phase towards which the paramagnetic phase can be unstable to, depends on the interaction strength, in contrast to the ordinary RPA. It numerically turns out that the \( \vec{k} \)-dependence of \( A_{\vec{k}} \) is enhanced by increasing the interaction strength. \( A_{\vec{k}} \) is typically largest for \( k = 0 \), and such is \( \chi_1(\vec{k}) \). The contribution involving \( A_2 \) is smallest, and has little influence on the magnetic properties. The numerous undefined symbols in Eqs. (2-3) can be gathered from Ref. [10], except for a misprint there: the third line of Eq. (A8) should read:

\begin{equation}
\frac{\partial^2 z}{\partial d'^2} = \frac{2\sqrt{2}p_0\eta}{1+\delta} \left( 2d + x + \frac{6xd^2}{1+\delta} \right).
\end{equation}

### III. RESULTS

We now proceed to the numerical results. We first calculate the density dependence of the static (but \( \vec{q} \)-dependent) magnetic susceptibility. In order to magnify the effect of \( t' \), we perform the calculation for \( t' = -0.47t \). Had we chosen \( t' = -0.5t \), then the van Hove singularity would lie right at the lower band edge. For \( U = 4t \) and \( \beta = 2 \) we display the density-dependence of \( \chi_s \) for several \( \vec{q} \)-vectors in Fig. [4]. For these parameters the paramagnetic phase does not show magnetic instability. At a particular doping the maximum of \( \chi_s \) (in its \( \vec{q} \)-dependence) tells us towards which phase an instability will develop. We checked numerically that this really happens at lower temperature. In the vicinity of half-filling \( \chi_s \)
is largest for the commensurate vector $Q = (\pi, \pi)$. In the low-density range $\chi_s$ is maximal for $q = 0$. This range is very large and extends from $\delta \simeq 0.38$ to $\delta = 1$, $\delta$ being the hole doping. In this domain the fluctuations are predominantly ferromagnetic, because the system is making use of the van Hove singularity to reduce its free energy. Between these two regimes there is a small window where the instability is towards an incommensurate phase with $\vec{q}$ along the diagonal of the Brillouin zone. We find that there is a value of the doping, that we denote $\delta_0$, beyond which $\chi_s$ is largest for $q = 0$. $\delta_0$ is seen to decrease with increasing interaction. We note that the doping $\delta_0$ at which $\chi_s$ is largest for $q = 0$ decreases with increasing interaction. For $U = 0$ we found it to be $\delta_0 = 0.42$, while for $U \geq 15t$ $\delta_0$ goes to zero. We thus obtain that, for strong coupling, the paramagnetic phase is unstable towards ferromagnetism over the entire doping range. This dependence of $\delta_0$ on $U$ can be traced back to the $q$-dependence of the effective interaction $A_{\vec{k}}$ entering Eq. (2), as discussed below Eq. (3). It turns out that the $q$-dependence is weak for weak coupling, and gets stronger with increasing $U$. This plays a crucial role in assessing towards which phase a magnetic instability may develop. We note that this effect is neglected in the usual RPA and in the two-particle self-consistent approach [14]. In those approaches all what matters is the $q$-dependence of the bare susceptibility $\chi_0$. We note that including $t'$ changes dramatically the phase diagram as compared to the $t' = 0$ case. In the latter case ferromagnetism may only show up for very strong coupling ($U \geq 66t$) and in a narrow doping region located around $\delta \simeq 15\%$ [13].

The influence of $t'$ on the doping dependence of the uniform susceptibility is displayed on Fig. 2 for $U = 4t$ and Fig. 3 for $U = 20t$. For moderate coupling decreasing $t'$ changes the monotonic behavior of $\chi_s(\delta)$ into a non-monotonic one, which is typical of high-$T_c$ materials. The height of the maximum increases with $t'$, and its location is shifted towards higher doping. This behavior, as well as the location and the height of the maximum, agree with the QMC data of Veilleux et al. [4]. We thus conclude that the non-monotonic behavior of $\chi_s$ for moderate coupling mostly results from band-structure effects. Experimentally the non-monotonic behavior of $\chi_S$ has been observed in La$_{2-x}$Sr$_x$CuO$_4$ and the maximum is reached for $x \simeq 0.25$ [10]; in YBa$_2$Cu$_3$O$_{7-x}$ $\chi_S$ only increases with increasing hole doping,
and one may assume that a maximum is reached for doping values that cannot be reached experimentally. According to Hybertsen et al. \cite{17}, $t' = -0.16t$ is relevant to La$_{2-x}$Sr$_x$CuO$_4$, in which case our approach yields the location of the maximum of $\chi_S$ at $\delta \simeq 0.20$. However the dependence of $\chi_S$ on $\delta$ is too weak to reproduce the experimental data. In the strong coupling regime $\chi_s$ has a maximum in its doping-dependence for $t' = 0$ \cite{18}. Decreasing $t'$ results into an enhancement of the maximum of $\chi_s$, and into a shift of it towards larger doping. For large $t'$ its location coincides with the van Hove singularity. Accordingly this non-monotonic behavior of $\chi_s$ for strong coupling results from a combination of interaction and band structure effects. We calculated $\chi_s(\vec{q})$ for other values of $\vec{q}$ too. For $t' = -0.47t$ it turned out that $\chi_s(\vec{q} = 0)$ is largest over the entire doping range. Thus raising up the interaction leads to a dramatic widening of the ferromagnetic domain. This is in agreement with the variational calculation of Pieri et al. \cite{4}, who investigated in more detail the low density route to ferromagnetism due to Müller-Hartmann \cite{4}.

We now turn to the charge structure factor. The latter is calculated according to Eq.(13) and Eq.(17) of Ref. \cite{10}. We recall that the comparison of the slave boson charge structure factor to existing QMC data displays a quantitative agreement. Here we perform the calculation for finite $t'$, for $U = 4t$, $\beta = 8$ and quarter-filling and display the result on Fig. 4. As compared to the $t' = 0$ result, decreasing $t'$ (i.e. $t'/t$ becoming increasingly negative) substantially suppresses the charge structure factor, especially around $(0, \pi)$, but also around $(\pi, \pi)$ for the largest $t'$. This suppression results from a frustration of the charge dynamics. We note that this suppression takes place in the parameter regime where the tendency towards magnetism is strongest. This leads us to propose that this is a general situation: frustrated charge dynamics and magnetic instabilities are occurring simultaneously in strongly correlated systems. This is well known for the Hubbard model at half-filling where the charge dynamics is so strongly frustrated that the system becomes insulating and the physics is dominated by strong anti-ferromagnetic fluctuations. Here the effect is less dramatic since the system remains metallic, but clearly noticeable. In the opposite case of a positive $t'$ (i.e. $t'/t > 0$) the charge structure factor gets essentially flat along the side
of the Brillouin zone. It is particularly enhanced in the vicinity \((0, \pi)\). This can be partly understood using a local picture. Assuming that the charges can form either a checkerboard or a stripe pattern, one sees that the number of frustrated bonds is larger for the former pattern. This plays little role if \(t'\) is negative, since one hop along the diagonal costs energy, but an increasingly important one when \(t'\) is increasingly positive. Clearly no such charge ordering occurs here, but tendencies towards such patterns emerge. The frustration effect is absent, and we indeed did not find any sign of a magnetic instability. The correlation frustrated charge dynamics-enhanced magnetic fluctuations can be traced back to the relationship between the local susceptibilities and the density

\[
\frac{1}{\beta} \sum_{\vec{k},i\nu_n} \left( \chi_S(\vec{k}, i\nu_n) + \chi_c(\vec{k}, i\nu_n) \right) = 2n ,
\]

which follows from the Pauli principle. Indeed if the local charge susceptibility is reduced, the magnetic one is enhanced, and \textit{vice versa}. In Fig. 5 we display the density dependence of the charge structure factor, for \(U = 4t, \beta = 8\) and \(t' = -0.47t\). Under an increase of the density, \(S_c\) first goes up, until \(\delta \approx 0.25\) and then goes down while going closer to half-filling. In weak coupling one would expect \(S_c\) to decrease upon doping, but the opposite behavior holds in a dense strongly correlated system.

In summary we studied the charge and magnetic properties of the 2-dimensional \(t-t'-U\) model. We found that a negative \(t'\) has a strong influence on the phase diagram, a very large portion of it being dominated by strong ferromagnetic fluctuations. We also showed that frustrated charge dynamics and strong magnetic fluctuations occur simultaneously. We found a tendency toward striped phases only for large positive \(t'\).

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FIG. 1. Doping-dependence of the magnetic susceptibility for $U = 4t$, $\beta = 2$ and $t' = -0.47t$ for a set of wave-vectors lying along the three main directions of the Brillouin zone. Inset: Doping-dependence of the magnetic susceptibility for $U = 0$ for the anti-ferro- and ferromagnetic wave-vector.
FIG. 2. Doping-dependence of the static and uniform magnetic susceptibility for $U = 4t$, $\beta = 3$ and $t' = -0.1t$, $t' = -0.3t$ and $t' = -0.47t$. 
FIG. 3. Doping-dependence of the static and uniform magnetic susceptibility for $U = 20t$, 
$\beta = 2$ and $t' = -0.1t$, $t' = -0.3t$ and $t' = -0.47t$. 
FIG. 4. Charge structure factor of the t-t'-U model at quarter filling, \( U = 4t \) and \( \beta = 8 \) and for several values of \( t' \).
FIG. 5. Charge structure factor of the t-t’-U model for $U = 4t$, $\beta = 8$ and $t' = -0.47t$ for several values of $\delta$. 