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Superconductivity, phase separation and charge transfer instability in the $U = \infty$ limit of the three band model of the CuO_2 planes

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The three band Hubbard model with nearest neighbour repulsion is studied in the $U = \infty$ limit using the slave boson technique and the large N expansion. A charge transfer (CT) instability is found like in weak coupling theory. The CT instability is always associated with a diverging compressibility leading to a phase separation. The total density and CT susceptibilities are analyzed in both the static and dynamic limit to gain insight on the strong mixing between the density fluctuations and the excitonic modes. The evaluation to order $\frac{1}{N}$ of the effective scattering amplitude in the Cooper channel shows the presence of superconducting instabilities in the s and d wave channel near the phase separation.

1. INTRODUCTION

The three band Hubbard model contains the essential ingredients in order to describe the CuO_2 planes of the superconducting oxides: an hopping term t depicts the strong hybridization between copper $d_{x^2-y^2}$ and oxygen p_x and p_y orbitals and a local repulsion U models the strong repulsion between holes on copper sites. This model can be reduced to an effective single band tJ model[1] which suitably describes the magnetic excitations. This reduction, however, is not allowed when a sizable nearest neighbor coulombic repulsion V between holes on copper and oxygen is present (extended Hubbard model). In fact the interaction V can soften the charge excitations leading to a physics different from the single band tJ model[2,3].

The three band extended Hubbard model has been analysed both in the weak (small V and U)[2] and in the strong coupling (small V and large U)[3] regimes, showing the following features: i) when V exceeds t the system undergoes a Charge-Transfer Instability (CTI); ii) because of the coupling of density fluctuations with the CT mode the presence of this CT instability, drives the system towards phase separation; iii) superconductivity (SC) can occur in the proximity of the unstable region.

However, whereas the SC instabilities in weak coupling are rather sensitive to the presence of U, in the strong coupling regime the Cooper channel instabilities survive the $U = \infty$ limit. Moreover, the strong coupling limit can capture some interesting physics related to the presence of a Metal-Insulator Transition (MIT). This transition is present in the real materials and could play a relevant role.

In the present work we focus our attention on the strong coupling regime by considering the limit $U = \infty$ of the three band extended Hubbard model. We use the slave boson trick and we carry out a controlled large N expansion using the functional integral technique. The physical copper hole creation operator is written as $d^{\dagger}_{i\sigma} = d^{\dagger}_{i\sigma} b_i$ and, as usual, a Lagrange multiplier λ_i is introduced to enforce the single occupancy constraint on copper. At mean field level ($N = \infty$) one can set the b_i and λ_i fields to their mean field values $b = \sqrt{N} r$ and λ respectively. It should be noted that, while b multiplicatively renormalizes the hopping integral t, leading to a reduction of the bandwidth, λ shifts the atomic d level: $\epsilon_d = \epsilon^0_d + \lambda$.

We decouple the copper-oxygen repulsion introducing two Hubbard-Stratonovich real fields X and Y. X is coupled to the difference in charge between a copper atom and its surrounding four oxygen orbitals and Y is coupled to the total charge of this cluster.

2. CHARGE TRANSFER INSTABILITY AND PHASE SEPARATION

The selfconsistent determination of the mean field values of the fields b, λ, X and Y leads to an effective band structure describing the coherent motion of quasiparticles forming a Fermi liquid with an effective optical p-d gap of the order $\Delta = \epsilon_p - \epsilon_d$ and an effective bandwidth $\sim r$. r vanishes at half-filling (one hole per unit cell) when the bare gap $\Delta_0 + 2V = \epsilon_p - \epsilon^0_d$ is larger than a critical value. There is a critical value V_c such that for $V > V_c$ this metal-charge transfer insulator transition becomes of the first order. In this case even at finite doping there is a line of first order transition between two metallic phases with dominant d character (at smaller doping) or dominant p character (at larger doping). This line ends with a critical point where the compressibility vanishes. However, this picture is only valid in the canonical ensamble (fixed doping). In the gran canonical ensamble a phase separation takes place (see below), which renders physically unaccessible the region around the above first order transition line.

The origin of the phase separation is the presence in the gran canonical ensamble of a CT instability coupled to a density instability. The CT instability corresponds to diverging p-d charge fluctuations and is described by the CT susceptibility $\chi \equiv \frac{\partial(n_p - n_d)}{\partial(\epsilon^0_d - \epsilon^0_p)}$ i.e. by the correlation function $\langle(n_p - n_d)(n_p - n_d)\rangle$ at zero frequency and momentum. A divergent χ is always accompanied by a divergent compressibility $\frac{dn}{d\mu} \equiv < (n_p + n_d)(n_p + n_d) >$. Because of this one can localize the CT instability by simply looking at the behaviour of the mean field solution for the chemical potential $\mu = \mu(\delta)$ as a function of doping. Since a divergent compressibility implies phase separation, the evaluation of μ vs δ is in any case necessary in order to carry out the standard Maxwell construction.

A typical result for the phase separation is shown in Fig. 1. The curve at which χ and $\frac{dn}{d\mu}$ diverge is also shown. Phase separation always occurs before the CT instability is reached. The continous line is the first order transition curve joining the MIT to the critical point (shown by the dot). In Fig. 1 we have fixed V=2.3 t and let Δ_0 vary. All energies are given in units of t.

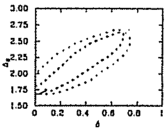

FIGURE 1

Fig. 1 Phase diagram Δ_0 vs δ for a value of V=2.3t. and in the presence of a O-O hopping $t_p = 0.2t$ and of a O-O local repulsion $U_p = 2t$. The diamond indicates the Brinkman-Rice transition point. The dashed line indicates the points at which χ and $\frac{dn}{d\mu}$ diverge; the continuous curve is the first order transition line between p and d metals.

Recently experimental evidence[4] has been reported of phase separation in $La_{2-x}Sr_xCuO_4$ between the superconducting and the large-doping metallic phases. Such an occurrence could be explained by the here considered model.

3. DYNAMICS OF THE CT MODE IN LARGE U

Within the joint slave boson-1/N expansion approach the extended Hubbard model is described by a Fermi liquid of interacting quasiparticles. In particular it is possible to define a scattering amplitude $\Gamma(\omega, q)$ (of order 1/N) and its usual dynamic and static limits Γ_ω and Γ_q which are related to the Landau Fermi liquid F_0^s factor, by the standard relations $F_0^s = N\rho_0\Gamma_\omega$ and $\Gamma_q = \Gamma_\omega/(1 + F_0^s)$ (ρ_0 is the density of states at the Fermi level). Whereas Γ_ω describes the effective interaction between the quasiparticles in the lowest (the only occupied) band resulting from bare interactions and interband processes, Γ_q is the static interaction once also the intraband screening is included. The diverging compressibility (with finite ρ_0 and $F_0^s = -1$) at the CT instability signals a negative, i.e. an attractive, Γ_ω.

Near the CT instability the static analysis revealed a strong coupling in the fluctuations of the conserved field $n_d + n_p$ and the non-conserved one $n_d - n_p$. The dynamic analysis in the q=0 limit singles out the purely CT mode so that the pole of the amplitude $\Gamma(\omega, q = 0)$ gives the energy of this mode at q=0. Close to the insulating region an analitic approach is possible expanding for small values of r. In this case it is possible to show that the CT mode has a large mass both in the absence and in the presence of V. The effect of V is to reduce slightly this mass, without sisably softening, however, the CT mode. The instability, instead, occurs as a consequence of the strong coupling (of order $1/r^3$ close to the insulating region) of this mode with the zero-sound (density-density) mode. The small reduction of the CT mass due to V results in a modification of the zero-sound velocity leading to damping first and then to instability with increasing V. Increasing r makes the softening of the CT mode more sizable in analogy with the weak coupling analysis.

It must be emphasized that the instability occurs without the vanishing of the CT mode mass.

4. SUPERCONDUCTIVITY

The effective total static interaction between the quasiparticles has also been studied in the particle-particle channel in order to establish the possibility of Cooper instabilities in the model. Its Fermi surface average (projected on s or d waves) gives the superconducting coupling constants $\lambda_{s,d}$. Negative values of the λ's are found in stable regions close to the phase separation.

The Coulomb interaction will rule out the phase separation favouring the presence of incommensurate charge-density waves. However the short range physics discussed above will be affected only at small momenta and frequencies. While it is possible that the intermediate q's behaviour will lead to sizable pairing within the static limit, a full analysis of the long range case requires the introduction of a dynamical screening and a subsequent solution of the Eliashberg equations.

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