Competing orders in the phase diagram of cuprate superconductors

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Abstract.

We perform self-consistent calculations in the framework of the Bogoliubov-deGennes theory with a model Hubbard Hamiltonian with strong local correlations. The calculations are performed in a charge density disordered system to study the competition of charge inhomogeneity, spin disorder and superconductivity. These calculations are appropriate to describe the cuprate superconductors’ phase diagram with the competition of different phases. We find that, in the presence of charge disorder the spin density wave (SDW) order occurs at higher temperatures above the opening of the superconducting gap. This is in opposition to the homogeneous systems where the SDW phase appears in the low doping compounds in the superconducting phase. These finding provides an explanation to the non-Fermi liquid behavior of the cuprates normal phase.

1. Introduction

The origin of the superconducting gap associated with the superconducting state and the relation to the pseudogap above the transition temperature ($T_c$) remains one of the central questions in high-$T_c$ research[1, 2]. The normal phase properties differs completely from the BCS superconductors. It is a matter of intense debate whether this problem is connected with the charge inhomogeneities observed in many different experiments[3, 4, 5, 6, 7, 8, 9, 10].

In order to obtain a unified interpretation to all of these observations we studied an electronic phase separation (EPS) transition that generates regions of low and high densities. Such a transition may be driven by the lower free energy of undoped antiferromagnetic (AF) regions[11] (intrinsic) or by the out of plane dopants[12] (extrinsic origin).

In this context we perform the study of the the superconducting (SC) and antiferromagnetic (AF) order in a model $t$-$t'$-$U$-$V$ Hamiltonian commonly used to describe the cuprates[13, 14] in an electronic disordered system. Chen and Ting[14] have studied this model for different doping and temperature and found that the AF is stronger at low doping and high temperatures. Self-consistent calculations in the Bogoliubov-deGennes (BdG) framework indicates that the AF order persists above the opening of the SC order parameter at very high temperatures. This is used to interpret the normal pseudogap phase, since this type of spin density wave will cause an additional scattering to the electrons and will change the Fermi liquid properties.
Figure 1. Typical phase separation calculation on a 105x105 square lattice with inhomogeneous densities represented by the color code[13, 11]. The BdG d-wave SC amplitude calculations are performed in a smaller 28x28 square lattice as drawn in the figure. The results are shown in the middle panel and yields $7 < \Delta_{\delta}(r_i) < 13\text{meV}$. On the right panel we show the local staggered magnetization $M_i$ along 28 points in row performed by the same calculation.

2. The model

The $t$-$t'$-$U$-$V$ Hamiltonian in a square lattice is defined as

$$
H = - \sum_{\langle ij \rangle \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\sigma} \langle \mu \rangle n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \frac{V}{2} \sum_{\langle ij \rangle \sigma'\sigma''} n_{i\sigma} n_{j\sigma'},
$$

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) is the usual fermionic creation (annihilation) operator at site $r_i$, with lattice parameter $a=1$ and spin $\sigma \{ \uparrow, \downarrow \}$. $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the density operator, and $t_{ij}$ is the hopping between sites $i$ and $j$. $U$ is the magnitude of the on-site repulsion, and $V$ is the magnitude of the nearest-neighbor attractive interaction. $\mu$ is the chemical potential. To apply the Bogoliubov-deGennes (BdG) approach we define the pairing amplitude $\Delta_{\delta}(r_i) = V \langle c_{i\delta} c_{i+\delta\uparrow} \rangle$, where $\delta = \pm \hat{x}, \pm \hat{y}$ are nearest neighbors unit vectors for a square lattice. The resulting effective Hamiltonian $H_{\text{eff}}$ is given by

$$
H_{\text{eff}} = - \sum_{i\delta\sigma} t_{i,i+\delta} c_{i\sigma}^\dagger c_{i+\delta\sigma} + \sum_{i\sigma} (\bar{\mu}_i) n_{i\sigma} + \sum_{i\delta} [\Delta_{\delta}(r_i) c_{i\delta} c_{i+\delta\uparrow} + \Delta_{\delta}(r_i) c_{i\delta}^\dagger c_{i+\delta\uparrow}^\dagger],
$$

where $\bar{\mu}_i = \mu - U/2 \langle n_i \rangle$ is the local chemical potential, which incorporates the site dependent Hartree shift $U/2 \langle n_i \rangle$ and the granular charge inhomogeneity of the system. The usual BdG equations for

$$
\begin{pmatrix}
K & \Delta \\
\Delta^* & -K^*
\end{pmatrix}
\begin{pmatrix}
u_{n\sigma}(r_i) \\
u_{s\sigma}(r_i)
\end{pmatrix} = E_n
\begin{pmatrix}
u_{n\sigma}(r_i) \\
u_{s\sigma}(r_i)
\end{pmatrix}
$$

with

$$
K u_{n\sigma}(r_i) = - \sum_{\delta} t_{i,i+\delta} u_{n\sigma}(r_{i+\delta}) + (\bar{\mu}_i) u_{n\sigma}(r_i),
$$

$$
\Delta u_{n\sigma}(r_i) = \sum_{\delta} \Delta_{\delta}(r_i) u_{n\sigma}(r_{i+\delta}) + \Delta_U(r_i) u_{n\sigma}(r_i),
$$

and

$$
\begin{pmatrix}
u_{s\sigma}(r_i) \\
u_{s\sigma}(r_i)
\end{pmatrix} =
$$
Figure 2. The calculated phase diagram showing the regions where the local staggered magnetization is different than zero and we call the SDW phase region. It starts at low temperature (blue curve) and ends at high temperature shown by the magenta line (high pseudogap line). The d-wave SC gap (GAP) onset temperature is shown by the green line (or low pseudogap line). The superconducting phase (SC) is the onset of phase coherence among the islands shown in Fig.1 (left panel).

and similar equations for $v_n(r_i)$. These equations give the quasiparticle eigenenergies $E_n(\geq 0)$. The BdG equations are solved self-consistently together with the $d_{x^2-y^2}$ pairing amplitudes

$$\Delta_{\delta}(r_i) = -\frac{V}{2} \sum_n [\mu_{n\sigma}(r_i)v^\sigma_n(r_i + \delta) + v^\sigma_n(r_i)\mu_{n\sigma}(r_i + \delta)] \tanh \frac{E_n}{2k_BT} , \quad (5)$$

and the inhomogeneous input (as shown in the left panel of Fig.1) hole density is given by

$$n(x_i)_\sigma = 1 - 2 \sum_n [||u_{n\sigma}(x_i)||^2 f_n + ||v_{n\sigma}(x_i)||^2 (1 - f_n)] , \quad (6)$$

The staggered magnetization $M_i = (-1)^\uparrow(n_{\uparrow} - n_{\downarrow})$.

We solved the above model self-consistently for the d-wave pairing amplitude $\Delta_{\delta}(r_i)$ for many values of doping level $p$ and temperature $T$, in order to study the phase diagram of cuprates. We used parameters close to the previous calculations of Chen and Ting for a homogeneous system, namely, $U=2.48t$, $t=1$ (0.15 eV) and nearest neighbors $t_{ij} = 0.25t$. $V$ varies from $1.4t$ at $n=0.90$ to $V=1.14t$ at $n=0.75$. This change in the two-body attractive potential is due to a phase segregation of the holes which forms islands of low and high densities. The holes get trapped in these grains, they loose kinetic energy what is a process that favors the pair attraction as discussed previously[13, 11, 15, 16]. Typical solutions of the local d-wave gap $\Delta_{\delta}(r_i)$ are shown in the middle panel of Fig.1.

3. Results and Conclusions

The EPS transition generates inhomogeneity in the (granular) local density $n_i$ that was simulated by the Cahn-Hilliard or time dependent Ginzburg-Landau approach[13, 11, 15, 16]. The result is a system
with grains or islands with characterized by low and high charge densities. In the BdG calculations we keep this granular structure fixed and use also the possibility that the attractive potential $V$ is scaled by the degree of disorder. In general, the self-consistent calculations yield non-zero values of the d-wave SC gap at temperatures well above $T_c$. This is shown by the green line in Fig.(2) or the onset of the $SDW + GAP$ phase region. For instance, for $p = 0.1$, the local gaps $\Delta_\delta(r_i)$ vanish near $T = 230K$. In this way the resistive transition at $T_c$ is estimated by the Josephson coupling among these regions[15, 16].

As mentioned, Chen and Ting[14] studied this model on homogeneous systems and found that the spin disorder or SDW phase starts near the optimum value using $U = 2.44t$ and $|V| = t$ at all doping and vanishes in the overdoped region. They identified the onset of SDW phase with the pseudogap temperature. We essentially generalized their calculations for the case of a system with disorder in the local charge density. In both the homogeneous and disordered system the local staggered magnetization $M_i$ depends strongly on the choice of parameters. The main purpose here is to show that the local SDW persists above $T_c$ at very high temperatures, close to the room temperature. The additional scattering from this spin disordered phase change the Fermi liquid properties and it is a possible interpretation of the cuprates normal phase. In this way we identify the high pseudogap line with the onset of staggered magnetization and the low pseudogap with the the onset of superconducting amplitudes $\Delta_d$. This last case is in agreement with various measurements connected with some superconducting properties like, for instance, the Nernst effect[17, 18].

Our results show a phase diagram more in agreement with the cuprates phase diagram[2] than that one calculated by Chen and Ting[14]. The difference is due to the charge disorder introduced as input in the self-consistent calculations. Therefore, our conclusion is that this local charge and spin disorder are important ingredients to study the different phases and crossover lines in the transport properties and phase diagram of cuprate superconductors.

4. Acknowledgments
This work was partially supported by the Brazilian agencies Faperj and CNPq.

5. References
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