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Appearance of antiferromagnetism and superconductivity in superconducting cuprates

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ABSTRACT

We represent the superconducting ceramic compounds by the single band extended Hubbard model. We use this model for solving the simultaneous presence of antiferromagnetism and the *d*-wave superconductivity in the Hartree–Fock (H–F) and in the coherent potential (CP) approximation, which is applied to the on-site Coulomb repulsion *U*.

The hopping interaction used in addition to the Coulomb repulsion causes rapid expansion of the band at carrier concentrations departing from unity. This expansion shifts the *d*-wave superconductivity away from the half filled point reducing its occupation range approximately to the experimental range in the YBaCuO compound.

The CP approximation used for the Coulomb repulsion is justified by the large ratio of Coulomb repulsion to the effective width of perturbed density of states being reduced by the hopping interaction.

The experimentally observed fast disappearance of antiferromagnetism is supported in calculations by the relatively large value of the total width of unperturbed density of states and the high values of the hopping interaction.

It is shown that our model is capable of describing the electron doped compounds as well.

1. Introduction

The coexistence of superconductivity (SC) and antiferromagnetism (AF) phenomena has been observed in many types of superconducting layered cuprates, such as $Nd_{2-x}Ce_xCuO_4$, $La_{2-x}Sr_xCuO_4$ [1,2] or $YBa_2Cu_3O_{6+x}$, in organic superconductors [3], in Uranium- and Cerium-based heavy-fermion systems [4], in Fe-based oxygen pnictide [5] and MFe_2As_2 family [6,7]. Transition between these two phases depends on carrier doping (by holes or electrons) and on external pressure. In layered cuprates, Fe-based oxygen pnictides, and the iron arsenide family, the superconducting and antiferromagnetic state can be suppressed by chemical doping. Almost all high-temperature superconducting cuprates at half-filling are antiferromagnetic insulators. Hole doping (in $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_{6+x}$) or electron doping ($Nd_{2-x}Ce_xCuO_4$) causes vanishing of the antiferromagnetic state and appearance of the superconducting state in the metallic state. The main difference between the hole-doped and electron-doped cuprates is in the range of the existing antiferromagnetic state. In the hole-doped cuprates, AF has already vanished at small doping (~0.03) and before the appearance of the SC state. In the electron-doped cuprates the AF state exists up to relatively high values of doping (~0.15), and the SC state rises before the AF state is extinguished. The schematic diagram for the hole-doped and electron-doped superconducting cuprates is shown in Fig. 1. The phase diagram of $YBa_2Cu_3O_{6+x}$ (as a function of carrier concentration) compound is very similar to the diagram of the $La_{2-x}Sr_xCuO_4$ compound after interchanging the dopant concentration to the hole number by the relation: $x = 1 - n$ (see e.g. [8]), and is shown in Fig. 6.

There are also numerous theoretical papers devoted to the problem of competition between AF and SC. Several methods are used to describe this phenomenon. The first attempts were carried out by use of the mean-field approximation [9–11]. Some authors use their computations by applying the dynamical mean-field theory (DMFT), which is based on the transition from the Hubbard model to the simple impurity Anderson model (SIAM) [12].

An early version of cluster DMFT was used by Lichtenstein and Katsnelson [13]. The authors found that *d*-wave superconductivity and antiferromagnetism coexist over most of the doping range. In their paper [14] the cellular dynamical mean-field theory (CDMFT) was used to compute zero-temperature properties of the two-dimensional square lattice Hubbard model (using the exact-diagonalization method). The authors have calculated the phase diagram that describes the competition between antiferromagnetism and superconductivity for both hole and electron doping at various values of *U*. They found, in general, homogeneous coexistence between AF and *d*-wave SC in the underdoped region (that feature

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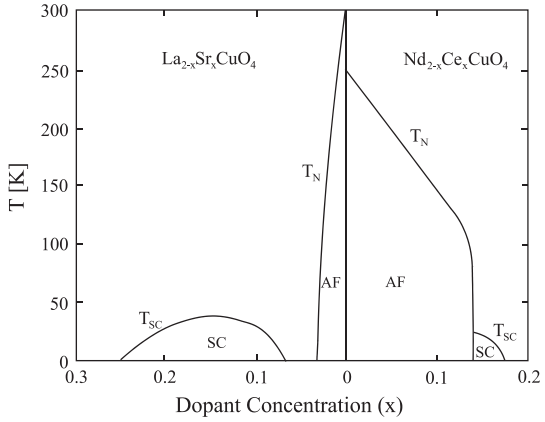

Fig. 1. Schematic phase diagram for both electron-doped ($Nd_{2-x}Ce_xCuO_{4-y}$) and hole-doped ($La_{2-x}Sr_xCuO_{4-y}$) superconductors, showing antiferromagnetic (AF) and superconducting (SC) phases.

is quite generally observed in quantum cluster methods, variational approaches, and mean-field theories that do not allow for spin or charge density modulations on large length scales). There is also another fully causal self-consistent method i.e. the dynamical cluster approximation (DCA) (see e.g. [15]). Using this method one can reduce the complexity of the lattice problem by mapping it to a finite-size cluster self-consistently embedded in a mean field. The main difference with their classical counterparts arises from the presence of quantum fluctuations. Mean-field theories for quantum systems with itinerant degrees of freedom cut off spatial fluctuations but take full account of temporal fluctuations. As a result the mean field is a time- or frequency dependent quantity.

Another methods use the spectral density approach [16]. The results obtained with the help of this method show the growing range of AF state with increasing U (the opposite behavior compared to the methods described earlier).

Despite the large progress in theoretical analysis of the coexistence between SC and AF there is still the need for description of experimental results. Particular attention should be devoted to decreasing the concentration range of coexistence between those two phases. Explaining the strong electron–hole asymmetry especially visible for the AF ordering (see Fig. 1) is also important.

The main objective of this paper is to explain the simultaneous appearance of AF and the d-type SC as shown by the diagram in Fig. 1, using the itinerant extended Hubbard model.

In our opinion this cannot be done by the simple Hubbard model with one interaction constant. The nature is too complicated to be described by such a model. Model which would bring such phases with one interaction constant only (even in high approximation) would suggest that almost everything can become SC and AF, what is a total absurd. The more realistic model requires several different interactions. Only the proper combination of those interactions can in some circumstances bring at some rare cases those rare phenomena. Therefore, the results obtained in the simple Hubbard model using higher approximations, which would reproduce together SC and AF experimental data would be false, since this would suggest that this rare phenomena would be quite popular. Our future work will concentrate on a model with higher level approximations but still the complicated physics of these phase transitions will imply that more than one interaction is responsible for them.

In Section 2 of the current paper we introduce the single band model Hamiltonian, which describes the CuO_2 plane in superconducting ceramics. We pay attention to the exchange hopping interaction, which is responsible for the change of the initial bandwidth. To describe magnetic properties of the system the crystal lattice is divided into two interpenetrating sub-lattices. Additionally the Hartree–Fock approximation is applied to all interactions (with an exception of Coulomb repulsion) appearing in the Hamiltonian. In Section 3 we present our numerical results. This section is divided into three subsections. The division of this section depends on the approximation used for Coulomb interaction (H–F or CPA). It also depends on the value of hopping interaction (whether it has nonzero value or not). We show the phase diagrams presenting the critical SC and AF temperatures versus carrier concentration. We also present the critical curves of the single site Hund's type exchange interaction responsible for creating an antiferromagnetic state. Finally, in Section 4 we conclude and summarize our results. This paper also includes two appendices, where we derived the equations for critical temperatures, carrier concentration and magnetic moment in the H–F and CP approximations for the case of coexisting d-wave SC and AF ordering. The calculations were performed using the equation of motion approach for the Green functions. To obtain the final results the moments method was used.

2. Model Hamiltonian

Our single band Hamiltonian has to represent the complex situation in the CuO_2 plane of layered compounds. Therefore it includes the on-site Coulomb repulsion U and the inter-site charge–charge interaction V. In addition we have the hopping interaction Δt (see [17–19]). This interaction causes the rapid growth of the bandwidth when the electron occupation n departs from unity. It stimulates the s type superconductivity (see [17,18]), which in our model is suppressed by the relatively strong effective Coulomb repulsion. The existing d-wave superconductivity (see [20–22]) is created by the negative inter-site charge–charge interaction V, and it is not hindered by the repulsion U. The concentration dependence of the effective bandwidth, $D(n)$, due to the nonzero value of Δt interaction, enhances the $U/D(n)$ ratio at growing occupation. This, in turn, in the CP approximation causes the repulsion of the d-wave SC state away from the half filled point. The model Hamiltonian used in our work is presented by:

$$H = -\sum_{\langle ij\rangle\sigma}[t - \Delta t(\hat{n}_{i-\sigma} + \hat{n}_{j-\sigma})]\, c^{+}_{i\sigma}c_{j\sigma} - \mu_0\sum_{i\sigma}\hat{n}_{i\sigma} + \frac{U}{2}\sum_{i\sigma}\hat{n}_{i\sigma}\hat{n}_{i-\sigma} + \frac{V}{2}\sum_{\langle ij\rangle}\hat{n}_i\hat{n}_j - F_{in}\sum_{i\sigma}n_\sigma\hat{n}_{i\sigma}, \quad (1)$$

where μ_0 is the chemical potential, $\hat{n}_{i\sigma} = c^{+}_{i\sigma}c_{i\sigma}$ is the electron number operator, $c^{+}_{i\sigma}(c_{i\sigma})$ creates (annihilates) an electron with spin σ on the i-th lattice site, $\hat{n}_i = \hat{n}_{i\sigma} + \hat{n}_{i-\sigma}$, and n_σ is the probability of finding the electron with spin σ in a band. Parameter t is the hopping amplitude for an electron of spin σ when both sites i and j are empty, and Δt is the hopping interaction. This interaction is defined as $\Delta t = t - t_1$, where t_1 is the hopping amplitude for an electron of spin σ when one of the sites i or j is occupied by an electron with opposite spin [20]. The single site Hund's type exchange interaction F_{in} added to the Hamiltonian can be interpreted as the interaction between electrons with parallel spins located on different orbitals of the multi-orbital single band Cu($3d$)–O($2p$) with two-dimensional character representing copper ceramic [23]. This magnetic interaction lowers the energy of each pair of electrons with parallel spins (does not matter up or down) with respect to antiparallel pairs.

The term: $\frac{V}{2}\sum_{\langle ij\rangle}\hat{n}_i\hat{n}_j$ is justified by the reduction of the three-band extended Hubbard model to the effective single-band model. In the three-band model the inter-band charge–charge interaction between holes on the oxygen orbitals $2p_{x,y}$ and on the copper levels $3d_{x^2-y^2}$ or $3d_{3z^2-r^2}$ (V_x and V_z) has the following form: