Inhomogeneities in superconductors: two component and two band scenarios

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Abstract. The scanning tunnelling microscopy experiments reveal nanoscale electronic inhomogeneities in superconducting materials as \textit{e.g.} \textit{Bi}\textsubscript{2}\textit{Sr}\textsubscript{2}\textit{CaCu}\textsubscript{2}\textit{O}\textsubscript{8+\delta}. In particular, large modulations in amplitude of the spectral gap in local density of states on a scale of a few lattice constants were observed. To understand recently discovered positive correlations between spatial modulations of the measured gap and positions of dopant atoms we use two component, respectively two band description of the material. Using real space Bogolubov-de Gennes equations, we calculate fluctuations of the pairing amplitude and order parameter, local density of states and Bogolubov angle. We discuss correlation between local characteristics of superconductor and note that the experimental data can be understood within the proposed models under reasonable assumptions.

1. Introduction

High temperature superconductors (HTS) still present a challenge and are the objects of intensive experimental [1] and theoretical studies [2]. Of particular interest are recent results obtained by means of scanning tunnelling microscopy [3] (STM). This technique probes local properties of materials with atomic precision. The most reliable data have been obtained for \textit{Bi}\textsubscript{2}\textit{Sr}\textsubscript{2}\textit{CaCu}\textsubscript{2}\textit{O}\textsubscript{8+\delta} family of HTS mainly due to the good quality of their cleaved surfaces. The experiments [4] reveal the existence of small scale (dimensions of few nanometers) inhomogeneities of the order parameter, positive correlation between positions of oxygen dopants and variation of the pairing amplitude [5] and even more advanced correlations [6] between local characteristics measured at different temperatures.

The two dimensional nature and very short coherence length makes the role of intrinsic disorder necessarily present in these doped Mott insulators very important [7]. Like in the previous theoretical work [8] we use the real space approach to calculate the local characteristics of the system. We shall study two different models of superconductivity with local pairing characteristics [9]. First is the two component model which we shall call boson-fermion model (BFM). BFM describes the system of fermions and bosons scattering with each other. It is this scattering which is responsible for superconducting ground state of the model [9, 10]. As the proper quantum chemical description of the electron spectrum in real materials always involves many orbitals [11] we shall also use two orbital model. The many orbital approach has been
argued to be important for HTSs [12]. In a two orbital BCS like model the local pairing of Hubbard negative $U$ variety has been assumed.

The main purpose of this paper is to show the potential and limitations of the above models to describe the observed by STM real space correlations. More detailed analysis and comparison with experiments will be presented elsewhere.

2. The models, approach and results

We use the following Hamiltonian of the boson-fermion model [9]

$$H^{BF} = -\sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i,\sigma} (V_i - \mu) c_{i\sigma}^\dagger c_{i\sigma} + \sum_i \left(E_i^B - 2\mu\right) b_i^\dagger b_i + \sum_{i,j} g_{ij} \left(b_i^\dagger c_{i1} c_{j1} + b_i c_{i1}^\dagger c_{j1}^\dagger\right),$$

where $i,j$ denote lattice sites of the square lattice, $c_{i\sigma}^\dagger, c_{i\sigma}$ ($b_i^\dagger, b_i$) stand for creation, respectively annihilation operators of fermion (boson) at the site $i$. $\sigma$ is spin index, $\mu$ denotes chemical potential and $t_{ij}$ are hopping integrals. We assume that the disorder in the sample modifies local positions of boson levels $E_i^B$ and introduces potential scattering centers $V_i$ for fermions. To proceed we shall decouple the interaction term in the mean field like approximation [13] and solve the resulting boson Hamiltonian exactly and the fermion one with help of canonical Bogolubov-Valatin transformation. The resulting Bogolubov-de Gennes equations are solved self-consistently at all sites of two dimensional $n \times m$ square lattice. It is important to remember that in this model bosonic $< b_i >$ and fermionic $\Delta_{ij}$ order parameters are proportional to each other and thus condensation in bosonic subsystem is accompanied by superconducting transition in fermionic one [14].

The general Hamiltonian of two orbital model reads

$$H = -\sum_{i,j,\lambda',\sigma} t_{ij} c_{i\lambda\sigma}^\dagger c_{j\lambda'\sigma} + \sum_{i,\lambda,\sigma} (\varepsilon_{\lambda} - \mu) c_{i\lambda\sigma}^\dagger c_{i\lambda\sigma} + \sum_{i,\lambda_1,\lambda_2,\lambda_3,\lambda_4} U_{i,\lambda_1\lambda_2\lambda_3\lambda_4} c_{i\lambda_1\sigma}^\dagger c_{i\lambda_21\sigma}^\dagger c_{i\lambda_3\sigma} c_{i\lambda_4\sigma}$$

in the same notation as above except that $\lambda = 1,2$ is an orbital index. In the two orbital model the disorder is assumed to cause the pair scattering $U_{i,\lambda_1\lambda_2\lambda_3\lambda_4}$.

The order parameters $\Delta_{i\lambda_1\lambda_2}(\vec{r}_i) = -\sum_{\lambda_3,\lambda_4} U_{i,\lambda_1\lambda_2\lambda_3\lambda_4} f_{\lambda_3\lambda_4}(\vec{r}_i)$, the (in general inter-orbital) pairing correlation functions $f_{\lambda_3\lambda_4}(\vec{r}_i) = \frac{1}{2} \sum_{k} (u_{\lambda_3\lambda_4}(\vec{r}_i) v_{\lambda_4}\lambda(\vec{r}_i)(1 - f_k) - u_{\lambda_4\lambda_3}(\vec{r}_i) v_{\lambda_3}\lambda(\vec{r}_i)f_k)$, Hartree term $V_{\lambda}(\vec{r}_m) = \frac{1}{2} \sum_{\lambda} U_{\lambda\lambda'\lambda''\lambda'''} n_{\lambda'}(\vec{r}_m)$ and local number density $n_{\lambda}(\vec{r}_i) = \sum_{k} (|u_{\lambda\lambda'}|^2 f_k + |v_{\lambda\lambda'}(\vec{r}_i)|^2 (1 - f_k))$ are expressed in terms of eigenvectors $u_{\lambda\lambda'}(\vec{r}_i)$ and $v_{\lambda\lambda'}(\vec{r}_i)$ and eigenvalues $E_k$ of BdG equations [15] and evaluated self-consistently. Here $f_k = (\exp(\beta E_k) + 1)^{-1}$ is the Fermi-Dirac distribution function and $\beta = 1/k_B T$.

The amplitudes $u_k(\vec{r}_i)$ and $v_k(\vec{r}_i)$ describe the mixing of particle and hole excitations in the superconducting state. In the normal state $u_k(\vec{r}_i) = 1$ and $u_k(\vec{r}_i) = 0$ for particle-like excitation and take on opposite values for hole-like excitations. Due to normalization of amplitudes the particle-hole mixing in the superconducting state can be characterized by an angle $\theta(\omega, \vec{r}_i)$, known as Bogolubov angle. $\theta(\omega, \vec{r}_i) = \arctan \left(\frac{|u(\omega, \vec{r}_i)|}{|v(\omega, \vec{r}_i)|}\right)$ with $u(\omega, \vec{r}_i)/v(\omega, \vec{r}_i)$ being a weighted average [16] of $u_k(\vec{r}_i)/v_k(\vec{r}_i)$ at energy $(+/-)\omega$.

We concentrate discussion of the results on few aspects related to inhomogeneities observed in superconductors. Our main assumption in this work is that the pairing interaction is intimately connected with impurities which open the boson-fermion scattering channel in the BFM and are the source of negative $U$ centers in the TBM. Thus in both cases we consider disorder in Cooper channel. The models, however, allow for much more subtle effects of impurities on the superconducting state.

In figure (1) we show temperature dependence of the bosonic order parameter as function of temperature calculated for two disconnected clusters of different value of $E_i^B = 0.0t$ or $0.45t$
Figure 1. Temperature dependence of average boson order parameter $|<b_i>|$ in the first (solid red) and second (dashed green) superconducting $7 \times 7$ cluster located in $17 \times 37$ system. In the left panel the clusters are 13 and in the right one 2 lattice sites apart. The insets show detailed view for temperatures close to $T_c$. In the first cluster $\bar{E}_B = 0.0$, while in second 0.45t.

Figure 2. Maps of the order parameter $|<\Delta_i>| = |\sum_j(-1)^{i+j}\Delta_{ij}|$ (left panel) in BFM for temperature $T = 0.0$ and system size $37 \times 41$ with d-wave symmetry and the Bogolubov angle at $\omega = 0.5t$ (right panel). Other parameters: $\bar{E}_B = 0.6t$, g=t, t=1.0. (all energies are measured in units of hopping t) placed in a nonsuperconducting host. If the distance between clusters is larger than the coherence length (left panel) the two gaps develop independently and there are two different transition temperatures. If the clusters are closer the two gaps still have different magnitude over the whole temperature range up to $T_c$. However, they both disappear at the same temperature $T_c$. In our local pairing model aimed at description of short coherence length superconductors this happens for the distance between clusters being of order of 2-3 lattice spacings as is seen in right panel of figure (1). Figure (2) shows the maps of the the local order parameter calculated within BFM for d-wave superconductor as a staggered sum over four bonds to nearest neighbor sites $|<\Delta_i>| = |\sum_j(-1)^{i+j}\Delta_{ij}|$ (left panel) and the local Bogolubov angle (right panel). Similar patterns visible in figures are to be expected as both the order parameter and Bogolubov angle are proportional to the amplitude $u_k(\vec{r}_i)$. It has been argued that this measure of the relative weight of particle and hole amplitudes can be deduced from comparative tunnelling measurements at positive and negative voltages [16].

We start the discussion of the results obtained in TBM with the remark that maps of local values of the order parameter $\Delta(\vec{r}_i)$ in band 1 and 2 (not shown) are similar despite different amplitudes of the two gaps. Due to short range paring interaction there is also very large positive correlation between the positions of impurities (negative U centers) and the value of the gap. The total and projected onto the bands local densities of states along the line X=7 are shown as function of energy in figure (3). The consecutive curves calculated at T=0K correspond to Y ranging from -13 up to 9. Marked in red are the curves for those values of Y, where U-centers exist, while blue are for sites without interaction. Note, however that the local density
of states at the sites without interaction show much higher coherence peaks (characteristic of a superconductor) than those obtained for a site with interaction. It is interesting that these features are mainly observed at the energies corresponding to the lower value of the two gaps.

In conclusion, our studies demonstrate the potential of both models to describe the observed correlations between various local properties of high temperature superconductors measured with STM. The sharp superconducting like features observed at sites with no attractive interaction are due to proximity and remind the effect discussed by Fang et al. [17]. The observation of similar features in STM spectra may indicate dependence of tunnelling matrix elements on orbitals and/or energy.

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Figure 3. The local density of states (left) and projected onto band 1 (middle) and band 2 (right) are plotted as function of energy along the X=7 line of our 21×27 s-wave superconductor. The red lines mark the positions of negative U centers: U_{11}=-3.5, U_{22}=-1.5, t=1.