Local properties of an inhomogeneous two-component correlated superconductor

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Abstract. The effect of random point-like impurities on correlated superconductor has been studied. We use the two component (also called boson-fermion (BF)) model formulated in a real space supplemented with strong on-site electron-electron repulsion U and solve it by means of the real space Bogoliubov-de Gennes approach. It has been shown that due to electron correlations the gap is larger near the impurity sites, contrary to the results for the same model but without U. This naturally leads to positive correlations between the gap magnitude and the position of impurities, as was observed in various scanning tunneling measurements performed on d-wave symmetry BSCCO-2122 superconductors. Strong correlations are responsible for the protection of the low energy quasiparticles against disorder.

1. Introduction

Strong correlations play a crucial role in high-temperature superconductors (HTS). They are commonly believed to be responsible for both the Mott insulating and the d-wave superconducting state. Disorder is introduced into the system in the process of doping and is unavoidable in these materials. Indeed, the recent scanning tunneling microscopy (STM) measurements have revealed nanoscale inhomogeneities in high temperature superconducting cuprates [1, 2]. It has also been observed in pnictide [3] superconductors. Detailed analysis of the results obtained in these experiments unveiled the unexpected correlation between positions of dopant oxygen atoms in $Bi_2Sr_2CaCuO_{8+\delta}$ systems and the large value of the gap. These positive correlations have been successfully analyzed in terms of $t-J$ [4] and boson-fermion [5] models of superconductivity.

Another important experimental fact about the superconducting state, at least in some HTSs is its apparent insensitivity to disorder [6], in marked contrast to conventional theories for d-wave pairing, which predict just the opposite [7]. Recently it has been shown that strong correlations may be responsible for this behavior [8]. In other words strong correlations make the d-wave superconductor described by the $t-J$ model robust against disorder. It is an interesting question if the same reasoning can be applied to Boson-Fermion model, i.e. if the addition of strong on-site repulsion between fermions in the boson - fermion mixture will also lead to renormalization of disorder effects and in particular to smearing of the low energy parts of the local densities of states as observed in experiment. To answer this question we use two component model [9] in its real space version [10] and study the local properties of materials with d-wave symmetry of the order parameter in the presence of 'atomic' disorder. This so called boson-fermion (BF) model has earlier been proposed by many groups [12] to describe HTS.
2. Model and approach

The boson-fermion model describes two kinds of quantum objects coexisting in the system - local electron pairs (hard-core bosons) and itinerant fermions - coupled with each other via mechanism of charge transfer. Hamiltonian of this two component model (in standard notation) has the form [5, 11]

\[ \hat{H}^{BF} = \sum_{i,j,\sigma} t_{ij} c_{i,\sigma}^{\dagger} c_{j,\sigma} + \sum_{i,\sigma} \left( V_i^{imp} - \mu \right) c_{i,\sigma}^{\dagger} c_{i,\sigma} + \sum_{i,\sigma} U c_{i,\sigma} c_{i,-\sigma} c_{i,-\sigma}^{\dagger} c_{i,\sigma}^{\dagger} + \sum_{i,j} \left( E_i^{BF} - 2\mu \right) b_i^{\dagger} b_j + \sum_{i,j} \frac{g_{ij}}{2} \left( b_i^{\dagger} (\hat{c}_{i,\uparrow} \hat{c}_{j,\downarrow} - \hat{c}_{i,\downarrow} \hat{c}_{j,\uparrow}) + h.c. \right). \]  

(1)

Third term in (1), with \( U > 0 \) describes electron-electron interaction. The interaction between fermions and charged bosons is provided by the coupling \( g_{ij} \), which for a d-wave symmetry takes form \( g_{ij} = g_0 \) for nearest neighbour sites \( \langle i, j \rangle \) only, positive along X-axis and negative along Y-axis.

If \( U \ll zt \) we shall use a mean field approximation. This approximation merely changes the local impurity potential in the above Hamiltonian \( V_i^{imp} \rightarrow \tilde{V}_i^{imp} = V_i^{imp} + 0.5 U n_i^{\uparrow} \). Due to the site dependence of both \( V_i^{imp} \) and \( n_i^{\uparrow} \) one expects some interplay of disorder and correlation even at this level of approximation. For \( U \gg zt \) the Gutzwiller approximation has been used. This approximation, which projects out doubly occupied sites leaves the on-site parameters unchanged but renormalizes hoping \( t_{ij} \) and electron-boson interaction \( g_{ij} \) as \( t_{ij} \rightarrow t_{ij} \tilde{r}_{ij} \) and \( g_{ij} \rightarrow \tilde{g}_{ij} = g_{ij} \tilde{r}_{ij}^0 \). The factors \( r_{ij}^0 \) and \( r_{ij}^0 \) are known as Gutzwiller renormalization factors [13] and for the present model they read

\[ r_{ij}^0 = r_{ij}^0 = \sqrt{\frac{2 \left( 1 - n_i^{\uparrow} \right)}{2 - n_i^{\uparrow}}} \sqrt{\frac{2 \left( 1 - n_j^{\uparrow} \right)}{2 - n_j^{\uparrow}}}. \]  

(2)

The boson-fermion Hamiltonian with correlations treated in mean field, respectively Gutzwiller, approximation can be written in a concise form as

\[ \hat{H}^{BF} = \sum_{i,j,\sigma} \tilde{t}_{ij} c_{i,\sigma}^{\dagger} c_{j,\sigma} + \sum_{i,\sigma} \left( \tilde{V}_i^{imp} - \mu \right) c_{i,\sigma}^{\dagger} c_{i,\sigma} + \sum_{i} \left( E_i^{BF} - 2\mu \right) b_i^{\dagger} b_i + \sum_{i,j} \frac{\tilde{g}_{ij}}{2} \left( b_i^{\dagger} (\hat{c}_{i,\uparrow} \hat{c}_{j,\downarrow} - \hat{c}_{i,\downarrow} \hat{c}_{j,\uparrow}) + h.c. \right). \]  

(3)

It still contains many body part describing charge exchange between both subsystems. The relevant parameters, however, have been changed as a result of strong electron-electron interaction. To decouple fermionic and bosonic degrees of freedom we use Hartree-Fock-Bogoliubov approximation \( b_i^{\dagger} (\hat{c}_{i,\uparrow} \hat{c}_{j,\downarrow} - \hat{c}_{i,\downarrow} \hat{c}_{j,\uparrow}) \simeq (b_i^{\dagger} \hat{c}_{i,\uparrow} \hat{c}_{j,\downarrow} - \hat{c}_{i,\downarrow} \hat{c}_{j,\uparrow}) + \hat{b}_i^{\dagger} (\hat{c}_{i,\uparrow} \hat{c}_{j,\downarrow} - \hat{c}_{i,\downarrow} \hat{c}_{j,\uparrow}) \). This leads to the decomposition of (3) onto the separate parts \( \hat{H}^{BF} = \hat{H}^B + \hat{H}^F \) with

\[ \hat{H}^B = \sum_{i} \left[ (E_i^{BF} - 2\mu) b_i^{\dagger} b_i + \chi_i b_i^{\dagger} b_i^{\dagger} \right], \]  

(4)

\[ \hat{H}^F = \sum_{i,j,\sigma} \left[ t_{ij} + \delta_{ij} \left( \tilde{V}_i^{imp} - \mu \right) \right] c_{i,\sigma}^{\dagger} c_{j,\sigma} + \sum_{i,j} \left[ \Delta_{ij} \left( \hat{c}_{i,\uparrow}^{\dagger} \hat{c}_{i,\uparrow} - \hat{c}_{i,\uparrow}^{\dagger} \hat{c}_{i,\uparrow} \right) + h.c. \right], \]  

(5)

where \( \chi_i = \sum_{\langle j \rangle} (\tilde{g}_{ij}/2) (\hat{c}_{i,\uparrow} \hat{c}_{j,\downarrow} - \hat{c}_{i,\downarrow} \hat{c}_{j,\uparrow}) \) and \( \Delta_{ij} = (\tilde{g}_{ij}/2) (\hat{b}_j) \).
Boson part of this problem is exactly solvable [5, 10, 11] by the means of standard statistical approach and we get

\[
\langle \hat{b}_i \rangle = -\frac{\chi_i}{2\epsilon_i} \tanh \left( \frac{\epsilon_i}{k_B T} \right),
\]

\[
\langle \hat{b}_i^\dagger \hat{b}_i \rangle = \frac{1}{2} - \left( \frac{E_i^B - 2\mu}{4\epsilon_i} \right) \tanh \left( \frac{\epsilon_i}{k_B T} \right),
\]

with \( \epsilon_i = \frac{1}{2} \sqrt{(E_i^B - 2\mu)^2 + 4|\chi_i|^2} \).

The fermion part \( \hat{H}^F \) has the standard BCS structure and could be diagonalized by the Bogoliubov-Valatin transformation. This results in the following Bogoliubov-de Gennes equations, with \( \Delta_{ij} = \Delta_{ij} + \Delta_{ji} \)

\[
\sum_j \left( \tilde{\tau}_{ij} + \left( \tilde{V}_i^0 - \mu \right) \delta_{ij} \right) \tilde{\Delta}_{ij} = -\tilde{\tau}_{ij} - \left( \tilde{V}_i^0 - \mu \right) \delta_{ij},
\]

solution of which enable us calculation of all parameters of interest. In particular the local density of states (LDOS) \( N_i(\omega) \) and local fermion number density \( n_f^l \) is found to be

\[
N_i(\omega) = \sum_l \left[ |u_l|^2 \delta(\omega - E_l) + |v_l|^2 \delta(\omega + E_l) \right],
\]

\[
n_f^l = \sum_l \left[ |u_l|^2 f(E_l) + |v_l|^2 (1 - f(E_l)) \right],
\]

where \( f(E_l) = 1/[\exp(E_l/k_B T) + 1] \) is the Fermi-Dirac distribution function.

The above equations are solved self-consistently on a finite cluster of size 31\times47. All energies are measured in units of nearest neighbour hoping \( t \) of homogeneous system. The next nearest neighbour hoping \( t' = -0.25t \). The position of the bosonic level \( E_i^B = 2\mu = 0.5t \), the interaction \( g_0 = 0.5t \) and total concentration of carriers \( n^{tot} = 0.9 \). We take point like impurities with the strength \( V_{imp} = 1t \) and varying concentration \( n_d \).

3. Results

To understand how correlations and disorder acting together affect the superconducting properties of the boson-fermion model we compare the results of the model without correlations to those with U. Figure 1 shows the evolution of spatially averaged density of states (DOS), defined as

\[
\langle N_i(\omega) \rangle = \sum_{x=1}^{L} N_i(\omega) (L \text{ is a total number of sites}) \text{ with the concentration of 'atomic' point-like impurities } V_{imp}.
\]

As one can notice, with increasing concentration of impurities in uncorrelated d-wave boson fermion model or if mean field approximation is used for weak correlations \( U = 1.0t \) the gap in DOS is losing its characteristic d-wave shape. The coherence features are smeared by impurities and their maxima only slightly move away of the chemical potential located at \( \omega = 0 \). With higher concentration of impurities there appear low energy (resonance) states which 'fill' the gap. As mentioned above the mean field approach to electron-electron interaction results in site dependent modification of the 'effective' potential \( V_{imp} \). For a given parameters the change is of the order of 10% and thus hardly seen in the figures. The low energy resonances are almost absent in the strong correlation limit \( U \to \infty \) (lower panels of Fig. 1)). In this case the gapless nodal quasiparticles are more robust against disorder, leading to the low-energy density of states that is quite insensitive to impurities. The structures seen
in the energy dependence of the density of states in all panels is related to the finite size of our system and its discrete energy spectrum. The asymmetry of the spectrum is related to the Van Hove singularity in the normal state density of states, which in the model with the present set of parameters lies below the chemical potential.

We also look how strong correlations affect local pairing amplitudes in a disordered superconductor. Figure (2) shows that in the absence of strong correlations (uncorrelated d-wave boson fermion model or a mean field treatment of Coulomb repulsion, left and middle panels) impurities reduce the value of the gap at the dopant sites and in a surrounding area. When a Gutzwiller approximation is applied (right panel) the value of the gap at the impurity sites is larger than the average value. It is obvious, that this gives simple explanation to the discovered positive correlation between the value of the spectral gap in the local density of states (LDOS) and the position of dopant atoms [2]. Uncorrelated boson-fermion model offers the explanation of this puzzling behavior under the assumption [5] that dopant impurities provide not only potential scattering but also change the positions of the bosonic levels. The strongly correlated impure boson-fermion model, in a close analogy with impure $t - J$ model [4], indicates the important role of impurity scattering in establishing the positive correlation between position of dopants and the value of the gap. It is thus a matter of future experiments to decide between various scenarios. Closer look at Fig.(2) shows that in uncorrelated system the response to the impurity spreads over a distance of few lattice constant, whereas in the correlated one it is highly localized in the close vicinity of the impurity site.
Figure 2. (Colour online) Maps of order parameter $\Delta_i = \sum_{<j>} |r_{ij}^2 \Delta_{ij}|$ in a system with $n_d = 10\%$ of potential impurities. Positions of dopant atoms are marked by green points. Left panel stands for uncorrelated d-wave boson fermion model. Middle panel present the results of the mean field approximation while right one the Gutzwiller approximation.

Figure 3. (Colour online) The local densities of states (LDOS) for sites along a cut through the lattice for $X = 5$. Left panel refers to uncorrelated d-wave boson fermion model and right one shows LDOS obtained within Gutzwiller approximation for a system with $n_d = 10\%$ of impurities. Energy dependence of LDOSs at impurity sites are plotted in green.

In the short coherence length superconductors the response to impurities obtained within Bogoliubov-de Gennes (BdG) approach differs considerably from the expectations of the standard Abrikosov-Gorkov theory [14, 15]. The BdG wave function distorts itself near the impurity site. In a weak scattering limit this distortion is similar for s- and d-wave symmetry of the order parameter. The strong correlations additionally protect the condensate against the disorder, at least at low energies. This leads to almost complete absence of impurity induced low energy excitations, in agreement with the results of scanning tunneling microscopy (STM) measurements [1, 2], where very low-energy spectra do not vary from one region of the sample to another.

In summary, our results elucidate the interplay between disorder and strong correlations. Even though we concentrate on the boson-fermion model some of the findings may have more general application. We have treated strong correlations by means of Gutzwiller approximation [13]. In disordered system it leads to random (but well defined) modifications of the hoping parameters and interactions. In the real space BdG approach the disorder is treated exactly. The protection of the low energy excitations against destructive impurity scattering we observe
here is similar to that earlier observed [8] for correlated $t - J$ model. The obtained results provide an explanation of the observed positive correlations between the value of the spectral gaps in the local density of states (LDOS) and the positions of dopant atoms [2]. The detailed analysis will be presented elsewhere.

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