The influence of strong diagonal disorder on superconductivity in the 2D attractive-U Hubbard model at low electron density

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Abstract. The properties of a two-dimensional low density (n<1) electron system with strong onsite Hubbard attraction U>W (W is the bandwidth) in the presence of a strong random potential V uniformly distributed in the range from -V to +V are considered. Electronic hoppings only at neighboring sites on the square lattice are taken into account, thus W=8t. The calculations were carried out for a lattice of 24x24 sites with periodic boundary conditions. In the framework of the Bogoliubov-de Gennes approach we observed an appearance of inhomogeneous state of spatially separated Fermi-Bose mixture of Cooper pairs and unpaired electrons with the formation of bosonic droplets of different size in the unpaired fermionic matrix. We observed an increase in the droplet size (from individual bielectronic pairs to larger droplets and finally to the percolation cluster) when we increase the electron density at fixed values of the Hubbard attraction and random potential.

1. Introduction

In present article, we consider two-dimensional attractive-U Hubbard model for an s-wave superconductor at low temperatures T in a strong random potential \[1-3\] and analyze this model in detail in the framework of the Bogoliubov-de Gennes (BdG) approach, taking into account both the solutions with positive energy values \(E_\sigma\) and the solutions with negative values of the energy of the electronic system \[4\]. Our goal is to observe how the amplitude of local pairing \(\Delta (r)\) changes spatially in the presence of disorder in the parameter ranges which have not yet been analyzed and correspond to strong Hubbard interaction \(|U|>W\) and strong diagonal disorder \(V>W\) at low electron densities \(n=0.125-0.3\). We also pursue a goal to study the effect of spatial inhomogeneities on physically relevant correlation functions.

2. Equations for inhomogeneous case and formulation of the model

We consider two-dimensional Hubbard model for an s-wave type disordered superconductor with short range (onsite) attraction between carriers, described by the Hamiltonian:

\[
H = -t \sum_{i,j,\sigma} \left( c^\dagger_{j,\sigma} c_{i,\sigma} + h.c. \right) - U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{i,\sigma} (V_i - \mu) n_{i\sigma}. \tag{1}
\]

Here, the first term describes kinetic energy, where \(t\) corresponds to hoppings to the neighboring sites of the square lattice, \(U=-|U|\) is the amplitude of the Hubbard attractive potential at one site,
\( \sigma \) are the creation (annihilation) operators for electron with spin \( \sigma \) at the square lattice site \( \mathbf{r}_i \), \( n_{i, \sigma} \) is the local electron density at site \( i \) for one component of the spin and \( \mu \) is the chemical potential. The random potential \( V_i \) is selected independently for each site and is governed by a uniform distribution in the range \([-V, V]\). Thus, \( V \) controls the intensity of diagonal disorder in the system. Introducing the Hartree-Fock shift of the chemical potential \( \mu = \mu - |U| n_i(\mathbf{r}_i) \), which depends on site \( i \), we write the BdG equations for the Bogoliubov functions \( u_n(\mathbf{r}_i), v_n(\mathbf{r}_i) \) participating in pairing [4]. Namely

\[
-\sum_{\pm \mathbf{x}, \pm \mathbf{y}} u_n(\mathbf{r}_i \pm \mathbf{x}, \pm \mathbf{y}) + (V_i - \mu_i) u_n(\mathbf{r}_i) + \Delta_n \cdot v_n(\mathbf{r}_i) = E_n \cdot u_n(\mathbf{r}_i); \tag{2}
\]

\[
\Delta_n^* \cdot u_n(\mathbf{r}_i) + \sum_{\pm \mathbf{x}, \pm \mathbf{y}} v_n(\mathbf{r}_i \pm \mathbf{x}, \pm \mathbf{y}) - (V_i - \mu_i) v_n(\mathbf{r}_i) = E_n \cdot v_n(\mathbf{r}_i). \tag{3}
\]

In the same time the pairing potential \( \Delta(\mathbf{r}_i) \) appearing in (2), (3), reads [4]:

\[
\Delta(\mathbf{r}_i) = U(\mathbf{r}_i) \equiv U \left[ \sum_n u_n(\mathbf{r}_i) v_n^*(\mathbf{r}_i) (1 - 2f_n) \right].
\]

Here \( E_n \) are the excitation energies in the system, \( \mu \) is the chemical potential in the presence of a random diagonal disorder \( V_i \), \( U(\mathbf{r}_i) \) is the mean field potential at the site \( \mathbf{r}_i \) [4], \( \Delta(\mathbf{r}_i) \) is the pairing potential at the site \( \mathbf{r}_i \) [4]. In order to take correctly into account both the pairing potential and chemical potential \( \mu \) in the system, which requires taking into account states below the Fermi level, we will keep the solutions of system (2), (3) with both positive energy values \( E_n \) and solutions with negative values of the energy of the electronic system, \( f_n = 1/\left[ \exp(E_n/kT) + 1 \right] \) is the Fermi-Dirac distribution function for a given value of the excitation energy \( E_n \). The chemical potential \( \mu \) is determined from the self-consistency condition for the density of particles \( n \) (which corresponds to the average number of electrons per site). We can effectively write down the normalization condition in the standard form

\[
\sum_n |u_n(\mathbf{r}_i)|^2 + \sum_n |v_n(\mathbf{r}_i)|^2 = 1.
\]

In (2), (3), in addition to the random potential \( V_i \), the mean field potential \( U(\mathbf{r}_i) \) at the site \( \mathbf{r}_i \) is included [4]. This yields

\[
U_i \equiv U(\mathbf{r}_i) = U \left[ \sum_n \left[ |u_n(\mathbf{r}_i)|^2 f_n + |v_n(\mathbf{r}_i)|^2 (1 - f_n) \right] \right].
\]

Starting from the initial assumption for \( \Delta_i(\mathbf{r}_i) \equiv \Delta_i \) and \( \mu \), we numerically solved the BdG equations (2, 3) for the eigenvalues \( E_n \) and the eigenvectors \( (u_n(\mathbf{r}_i)), (v_n(\mathbf{r}_i)) \) on a finite 2D lattice of \( N \times N \) sites with the periodic boundary conditions. Then we calculated the magnitudes of the amplitudes \( (u_n(\mathbf{r}_i)), (v_n(\mathbf{r}_i)) \) at the specific sites at low temperatures. Next, we calculated the local pairing amplitude \( \Delta(\mathbf{r}_i) = U \sum_n u_n(\mathbf{r}_i) v_n^*(\mathbf{r}_i) (1 - 2f_n) \) at each site and the density values of the types u and v at
the sites \( r_i \). We repeated the iteration process until the self-consistency for \( \Delta_i \) and \( n_i \) at each site was achieved.

3. The method of the calculations
Model (1-3) was studied for the parameter range \( 1 \leq |U| / t \leq 10 \) and \( 0 \leq V / t \leq 12 \) on a lattice with \( N = 24 \times 24 \) nodes. The study also considers low concentrations \( n = 0.125 \) at low temperatures. The value of the energy gap \( E_{\text{gap}} \) is defined as the smallest positive eigenvalue of the energy. Correspondingly \( \Delta_i \) is the value of the order parameter at the i-th site, \( V \) is the disorder amplitude.

The values of \( E_{\text{gap}} \) and \( \Delta_{\text{op}} \), as well as all the results, unless otherwise specified, were averaged over 25 launches with various random disorder distributions.

4. Trends in the system with moderate disorder when we increase \(|U|\)
The first version of the calculations in the framework of BdG equations (1-2) was performed at a temperature close to zero on the grid of \( N = 24 \times 24 \) sites, at extremely low electron concentration \( n = 0.15 \), and in the limit of very strong attraction between the electrons \( |U| = 10t \). The calculations were performed for moderate disorder \( V = 2 \). Figure 1 shows the trends manifested with an increase in \(|U|\) arising in the dependences of the spatial distribution of the electron density (left column), of the electron gap \( \Delta \) (right column). The distribution of all the quantities with increasing \(|U|\) (localized at individual sites) is shown below:

![Spatial distribution of electron gap and density](image)

Fig. 1. Spatial distribution of the electron gap \( \Delta \) (bottom line), electron density (upper line). The left column corresponds to \(|U| = 2t\), \( V = 2t \), middle column corresponds to \(|U| = 4t\), \( V = 2t \), right column corresponds to \(|U| = 10t\), \( V = 2t \). The calculations were performed for low electron density \( n = 0.15 \).

As we can see from Fig. 1, at low electron concentrations \( n = 0.15 \), the system even at moderate values of disorder tends to form droplets of the order parameter, the spatial arrangement of which correlates with the spatial distribution of electron density in the system (right column), as well as with a value characterizing the coexistence of holes and electrons in real space. The electrons in the system are located in the regions with small values of disorder. The system is not an insulator under the considered parameters, since the distribution of electrons in space has not split into separate isolated regions. At low concentrations, the system exhibits the properties of a bosonic metal, the carriers of which are bosonic clusters consisting of several electron pairs, each of which is a boson.
To characterize the relative localization of pairs in Fig. 2 we show the graphs of the dependence of the correlator \( \langle c_i^+ c_j c_i^+ c_j \rangle \), which is responsible for the transfer of pairs, on the distance as a function of concentration for given \(|U|\) and \(V\). In the above calculations, we did not average the disorder configurations, all the results are presented for one disorder implementation.

Fig. 2. The dependence of the mathematical expectation of \( \Delta \Delta \), which reflects the spatial distribution of electron pairs, on the distance between the pairs, expressed in terms of the lattice constants. A graph is presented with the average concentration \(n = 0.7\) for \(V = 8t\) and \(|U| = 6t\).

As we can see from Fig. 2, the concentration value \(n = 0.31\) corresponds to the proximity of the system to the transition to the state without pairing of electrons at all (with the pair parameter disappearing simultaneously at all sites). From Fig. 2 it follows that at all the values of electron’s concentration, a long-range order is established in the system, so that the pairs located at a maximum distance from one another prevail (Fig. 2). An analysis of the behavior of the pair correlator (Fig. 2), which is responsible for the spatial distribution of pairs in the system, does not allow us to conclude that at these parameters the system is an insulator. We believe that in this section we have indicated certain limiting values of the parameters corresponding to the transition of the system to the state of the insulator.

5. Calculations for extremely low densities and weak disorder
Calculations for the previously unexplored region of extremely low electron concentration \(n = 0.125\), were performed at a nonzero temperature on the grid of \(N = 24 \times 24\) sites for \(|U| = 10t\). The results of the previous section are supplemented by calculations for weak disorder with amplitudes \(V = 0.25t; 2t; 4.0t; 10.0t\). For \(|U| = 10t\) and \(V = 2t\), a series of figures (Fig. 3) shows how an increase in the concentration \(n\) affects the character and scale of the decrease in the average pairing parameter \(\Delta_{op}\) and the gap value \(E_{gap}\) with a concentration \(n = 0.18\) to \(n = 0.125\). Results are averaged over five configurations.

Fig. 3. a. Dependence of \(E_{gap}\) on the amplitude of the disorder \(V\); b. Dependence of \(\Delta_{op}\) on the amplitude of the disorder \(V\). \(n = 0.125\), \(|U| / t = 8\) for the lattice with \(24 \times 24\) sites.

The presence of a minimum in the dependence of the \(E_{gap}\) on the disorder degree \(V\) (Fig. 3.a) is consistent with the results from [8–10].

6. Calculations for low electron concentration, in the range of disorder from low to high value
This section presents the results of the calculations in a wide range of the degree of disorder with the amplitudes \(V = 0.5t; 6.0t; 10.0t\) for a \(24 \times 24\) system with a density of \(n = 0.15\).
Figure 4 shows that up to certain values of $V$ (of the order of $5t$), the correlations between the left and middle columns are clearly traced. Figure 4 shows the transition from the droplets of the order parameter to individual electron pairs - bosons with increasing disorder degree in the system. The question concerning the limiting value of the disorder at which our system passes from the Bose metal to the insulator in Fig. 4 remains open and requires additional investigation. Thus, our problem is divided into two independent problems: the Bose - metal problem and the insulator problem for the values of disorder exceeding the critical value, with dispersed droplets of the order parameter containing Bose states. From Fig. 5 c, from a comparison of all three columns, we can conclude that there is also a phase in which most of the electron pairs are localized, with a minority of delocalized pairs moving against the background of such Bose insulating state. Figure 5 shows the values of $v_{r} + v_{i}$ with the positive energy values for the first three excitations for a value $V = 4t$.

Fig. 5. The first three excitations are shown for the set of values $V = 4t; |U| = 6t, T = 0.01, n = 0.15$ (bottom row). From left to right, the excitation number for a given value of $|U|$ increases, having energies of 0.102606t, 0.172969t, 0.217828t.

7. Calculations for a high degree of disorder in the range of electron concentration from low $n = 0.15$ to average values $n = 0.32$

This section presents the results of the calculations in the range of electron densities from low $n = 0.15$ to moderate values $n = 0.30$ for the disorder amplitude of $V = 8t$ and Hubbard amplitude $|U|=6t$ for a lattice with 24x24 sites. Separate random excitations are also shown.

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**Fig. 4** Two-dimensional distribution of the electron density (left column), and order parameter (right column) for $n = 0.15, |U| / t = 6$, on the $24 \times 24$ lattice with disorder amplitude $a$ - upper line: $V / t = 0.5$; $c$ - the bottom line $V / t = 10.0$. 
As we can see, for the density \( n = 0.11 \), single pairs or doubled pairs of electrons (quartets) are observed on adjacent cells (Fig. 6), while at \( n = 0.17 \), larger droplets of the order parameter are observed (Fig. 6, 7). Droplets of the order parameter merge into the network of chains resembling the percolating cluster in the form of the tree with a lot of branches (Fig. 7), which practically do not experience discontinuities along their length. At \( n = 0.30 \) the resulting network of the order parameter in this case is concentrated in the spatial regions - the “valleys” between the peaks of the electron density (Fig. 7).

8. Conclusions
As the disorder grows, the spatial distribution of the local pairing amplitude \( \Delta(r) \) first takes the form of individual droplets, and then takes the form of individual pairs. Our results show, that when we increase the density, at first the transition from single electron pairs to larger droplets (containing larger number of pairs) takes place. And than finally a large percolating network of paired chains is formed in our system manifesting percolative phase-transition from granular to SC state.

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