Theory of superconducting pairing near the mobility edge

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We develop a theory of a pseudogap state appearing near the superconductor-insulator transition in strongly disordered metals with attractive interaction. We show that such an interaction combined with the fractal nature of the single particle wave functions near the mobility edge leads to an anomalously large single particle gap in the superconducting state near SI transition that persists and even increases in the insulating state long after the superconductivity is destroyed. We give analytic expressions for the value of the pseudogap in terms of the inverse participation ratio of the corresponding localization problem.

A rapidly growing number of experiments on various disordered superconductors show that a novel phase appears in the vicinity of the superconductor-insulator transition as sketched in the low temperature phase diagram in Fig. 1. On the superconducting side of the transition a relatively small magnetic field suppresses the superconductivity leading to an insulator characterized by a large thermally assisted resistance with a hard gap. Upon a further increase of the magnetic field the resistance and the gap drop\textsuperscript{1,5,6,7,8}. It is tempting to explain these data by a formation of localized Cooper pairs – in this picture the superconductivity is due to a fragile coherence between localized Cooper pairs, while the energy of single electron excitations is much larger and remains finite even when the coherence (and thus the superconductivity) is destroyed. Experimentally, this behavior is observed only for a limited range of disorder strengths, $\sigma_1 < \sigma < \sigma_2$, characterized by the conductivity $\sigma$ at room temperature. At weaker disorder, $\sigma \geq \sigma_2$, the destruction of superconductivity by a magnetic field leads, as usual, to a formation of a normal metallic state without any noticeable localization effects. At larger disorder $\sigma < \sigma_1$ superconductivity is replaced by a gapped insulator even at $B = 0$. Usual insulator with a variable-range hopping conductance is recovered at larger disorder, $\sigma < \sigma_0$.

The hypothesis of preformed Cooper pairs is further confirmed by the behavior of disordered superconductors at higher temperatures. On the insulating side of the transition in thick (effectively 3D) films one observes\textsuperscript{3,4,6,7,8,9} Arrenius behavior, $R(T) \propto \exp(T_1/T)$, at low temperatures. The experimental value of the activation energy, $T_1$, is somewhat larger than the superconducting gap in less disordered samples and grows with the disorder. For instance in InO\textsubscript{x} films $T_1 = 2 - 15$ K, while the critical temperature $T_c = 3.3$ K in best samples\textsuperscript{10,11}. However, at higher temperatures ($T \geq 10$ K for InO\textsubscript{x} films studied in Ref. [3] this behavior is replaced by Mott’s variable range hopping $R(T) \sim \exp(T_M/T)^{1/4}$. Thus, qualitatively the temperature plays the same role as the magnetic field, suppressing an unconventional insulator formed near superconductor-insulator transition. This can be easily understood if the insulating pseudogap is due to preformed Cooper pairs with a pairing energy somewhat larger than the superconductive gap in a less disordered samples.

The purpose of this Letter is to provide a justification for this picture and to construct the theory of localized Cooper pairs starting from a semi-microscopic model that contains only low energy electrons with BCS-type attraction and a strong random potential which leads to Anderson localization of single-particle states. An important ingredient of the problem is the fractal structure of single-particle wave functions, which sets in on a microscopic scale $L_0$ determined by the disorder potential and extends to the localization length $L_{\text{loc}}$.

It is well established that disorder has little effect on conventional superconductivity\textsuperscript{12,13} in the absence of Coulomb repulsion. On the mean-field level (neglect-
underdoped cuprates

underdoped cuprates

gaped insulating state similar to the one observed in

empted (upon
deformation). In each grain, the superconducting phase transition is pre-
duced by localization of electron wave functions provided that




events (grains) of size $L_{\text{loc}}$. In the
due to the fractal nature of the wave functions near the mobility edge $V_{\text{eff}} \sim L_{\text{loc}}^3(L_{\text{loc}}/L_0)^{D_2}$, where

′′inverse participation ratios′′ (IPRs),

as $\bar{\lambda}/(\nu_0 V_{\text{eff}})$. It is crucial for the following that this volume is parametrically smaller than the 'localization volume' $L_{\text{loc}}^3$ due to the fractal nature of the wave functions near the mobility edge $V_{\text{eff}} \sim L_{\text{loc}}^3(L_{\text{loc}}/L_0)^{D_2}$, where $D_2 < 3$, cf. 17,18. Then the energy scale $\Delta_1$ is parameterically larger than $\delta_L$. Thus, the strength of the disorder is characterized by two relevant energy scales, $\delta_L$ and $\Delta_1$.

Here we focus on two limiting cases

\[ \Delta \ll \delta_L \ll \omega_D \]  
\[ \delta_L \ll \Delta \ll \Delta_1 \]  

As shown below in the first regime the single-particle gap remains large leading to a gapped insulator. In the second regime the superconductivity persists, but the single-particle gap $\Delta_1$ is much larger than in conventional superconductors. In particular, the ratio of this gap to $T_c$ can be anomalously large. Moreover, in the latter regime the superconducting phase transition is pre-

empted (upon $T$ decrease) by a formation of a "pseudogapped" insulating state similar to the one observed in underdoped cuprates. 19

We assume that a BCS-type attraction between electrons at high energy scales $\sim \omega_D$ is only weakly affected by localization of electron wave functions provided that $\delta_L \ll \omega_D$. The theoretical reason for this is the scaling argument that says that physics at short scales and large energies is not affected by localization as long as $k_F L_{\text{loc}} \gg 1$. This is further collaborated by an experimental observation that $T_c$ changes little until one gets into a deeply localized regime. In a ferrom system with weak attraction one can leave only the pair interaction terms in the Hamiltonian leading to the usual BCS model in the basis of localized electron states:

\begin{equation}
H = \sum_{j\sigma} \epsilon_j c_{j\sigma}^\dagger c_{j\sigma} - \frac{1}{\nu_0} \sum_{j,k} \lambda_{jk} M_{jk} c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger c_{k\downarrow} c_{k\uparrow} \tag{3}
\end{equation}

where $\epsilon_j$ is the single-particle energy of the state $j$ and the matrix elements $M_{jk} = \int d\mathbf{r} \psi_j^\dagger(\mathbf{r}) \psi_k^2(\mathbf{r})$. In Hamiltonian

(3) we will also distinguish the off-diagonal dimensionless coupling constant $\lambda_{jk} = \lambda$ for $j \neq k$ from the diagonal one $\lambda_{jj} = \bar{\lambda}$ for the reasons detailed below.

To study the model (3) we need the statistics of single electron states near the 3D Anderson mobility edge. We expect that on average off-diagonal matrix elements, $M_{jk}$ with $j \neq k$ have the usual scaling $1/L_{\text{loc}}^3$ for the states localized at distances smaller than $L_{\text{loc}}$ from each other. In other words we assume that correlations $M_{jk}$ between wave functions of different states are much smaller than individual "inverse participation ratios" (IPRs), $M_{jj} = \int d\mathbf{r} \psi_j^2(\mathbf{r})$, which have the meaning of the inverse volumes of localized states, $V_{\text{eff}}$. In fact, extensive numerical studies 17,18 show that a typical IPR, $M$, scales as $M \approx L_0^{-3} (L_{\text{loc}}/L_0)^{-D_2}$, with $D_2 = 1.30 \pm 0.05$.

As discussed above, the thermodynamics of this model should be similar to a collection of grains of size $L_{\text{loc}}$ with Hamiltonians

\begin{equation}
H = \sum_{j\sigma} \epsilon_j c_{j\sigma}^\dagger c_{j\sigma} - \sum_{j,k} g_{jk} c_{j\uparrow}^\dagger c_{j\downarrow} c_{k\downarrow} c_{k\uparrow} \tag{4}
\end{equation}

where the average level spacing is $\langle \epsilon_{j+1} - \epsilon_j \rangle = \delta_L$, the off-diagonal part of the interaction has the usual form for a grain, $g_{jk} = g = \bar{\lambda} \delta_{jk}$ for $j \neq k$, while the diagonal part has an extra term $G$ so that $g_{jj} = g + G = \bar{\lambda} (L_{\text{loc}}/L_0)^{-D_2} / (\nu_0 L_0^3)$ due to the fractal nature of the wavefunctions.

We have checked that the results described in this Letter are the same (up to numerical factors of order one) for models (3) and (4).

We begin with the insulating region (1) where Cooper interaction can be treated perturbatively. 20 In the first order perturbation theory the minimum energy (counted from the chemical potential), $\Delta_1$, required to add a single electron to the system is

\begin{equation}
\Delta_1 = \frac{\bar{\lambda}}{2 \nu_0 L_0^3 (L_{\text{loc}}/L_0)^{D_2}} \tag{5}
\end{equation}

The coupling constant $\bar{\lambda}$ appearing in this equation is not renormalized by Cooper loops: indeed, the Hamiltonians (3) and (4) do not mix unoccupied and doubly occupied (unblocked) states with singly occupied (blocked) ones. Blocked states do not participate in pair scattering and contribute only their single-particle energy to the Hamiltonian. The additional contribution coming from the diagonal term in (1) is $G N_{\text{pairs}}$, where $N_{\text{pairs}}$ is the total number of pairs. Using the fact that the total number of electrons is $2 N_{\text{pairs}} + N_B$, where $N_B$ is the number of blocked states and shifting single-particle levels $\epsilon_j \rightarrow \epsilon_j + G/2$, we can rewrite Hamiltonian (1) as

\begin{equation}
H = \sum_{j\sigma} \epsilon_j c_{j\sigma}^\dagger c_{j\sigma} - g \sum_{j,k} c_{j\uparrow}^\dagger c_{j\downarrow} c_{k\downarrow} c_{k\uparrow} + \sum_{k} \left( \epsilon_k + \frac{G}{2} \right) \tag{6}
\end{equation}

Here the first two terms act only on unblocked states, while the summation in the last term is over decoupled blocked states. The renormalization affects only the interacting part which is of a standard BCS form. This
statement is valid for the reduced Hamiltonians \(3,4\) which contain pair-wise eigenstates only. In general, one would say that our phenomenological Hamiltonians \(3,4\) contain two different coupling constants originating from the competition between Coulomb and electron-phonon interactions – standard BCS coupling \(\lambda\) and the additional "diagonal" one, \(\tilde{\lambda}\), which characterizes interaction of two electrons in the same localized state.

Applying the same arguments to the Hamiltonian \(3,4\), we get a single-particle gap that varies from one level to another: \(\Delta^j = \tilde{\lambda} M_{jj} / (2\nu_0)\). The average density of single electron states in a large sample is controlled by the IPR distribution \(P(M)\):

\[
\nu(\varepsilon) = \nu_0 \int_0^{2\varepsilon \nu_0 / \tilde{\lambda}} P(M) dM
\]

Scaling theory of localization predicts that near the mobility edge \(P(M)\) acquires a scale-invariant form and this is indeed what was observed in numerical studies.\(^{15}\) Moreover, these data indicate that the distribution \(P(M)\) decreases fast at \(M / \bar{M} \rightarrow 0\) so that extended states occur too rare to smear up a gap-like behavior in the density of states \(7\) with the gap value given by Eq. \(5\).

We emphasize that the DoS \(7\) does not contain any "coherence peak" above the gap. The same qualitative behavior of the DoS in the insulating region was obtained by solving numerically BCS mean field equations for the disordered "negative-U" Hubbard model. Evidently, the spectral gap \(\Delta_1\) should be associated with the experimentally determined activation energy \(T_1\). The gap dependence \(5\) predicts a moderate increase \((\propto 1 / L_{D_2}/)\) of \(T_1\) with disorder strength in a complete agreement with the experimental data, see Fig. 2. Note that attempts to fit the data with a gap that scales as \(\delta_L \propto 1 / L_{loc}^{1}\) have failed spectacularly.\(^{21}\)

![FIG. 2: Experimental values of the gap, \(T_1\) (boxes) and a fit to the equation \(5\) with \(L_{loc} \sim (\sigma - \sigma_c)^{-1}\) that involved only the overall scale adjustment.\(^{22}\)](image)

We now turn to the parameter region \(2\) where one expects a global superconductive coherence. Namely, the condition \(\delta_L \ll \Delta\) assures that a large number of eigenstates \(\psi_j\) with energies down to \(\varepsilon_j \sim \Delta\) overlap significantly in the real space, so one can use the standard BCS-type self-consistent gap equation as first argued in Ref. \(11\).

However, due to an extra cost of creating an unpaired electron, the energy required to add an electron in this regime is no longer equal to the self-consistent gap \(\Delta\) as in the usual BCS theory. Indeed, because the addition of an electron increases the number of blocked states in \(M\) by one, we have

\[
\Delta_1 = \Delta + \frac{G}{2} \approx \Delta + \frac{\lambda}{2\nu_0 L_0^2 (L_{loc} / L_0)^{D_2}}
\]

In order to evaluate the energy of pair excitations, i.e., the excitations of the condensate with no unpaired electrons, it is convenient to rewrite Hamiltonian \(3\) in terms of Anderson’s pseudospin-1/2 operators\(^{21,22}\) defined on the subspace of unblocked states as \(s_j^+ = c_j^\dagger c_{j+} = (s_j^-)^\dagger\) and \(2s_j^z = c_j^\dagger c_j + c_j^\dagger c_{j-} - 1\). We have

\[
H = \sum_j \delta_j s_j^z - g \sum_{j,k} s_j^z s_k^z + \sum_B \left( \nu_B + \frac{G}{2} \right)
\]

In the BCS mean-field approximation eigenstates of \(4\) correspond to all spins being parallel or antiparallel to the effective magnetic field \(\hat{B}_j = -(2\Delta, 0, 2\varepsilon_j)\), where \(\Delta = g \sum_j (s_j^z)\), leading to a self-consistency condition

\[
\frac{2}{g} = \sum_j \frac{\varepsilon_j}{\sqrt{\varepsilon_j^2 + \Delta^2}}
\]

where \(\varepsilon_j = 1\) if the spin is against the magnetic field and \(\varepsilon_j = -1\) otherwise.

In the ground state all spins are along their magnetic fields, \(\varepsilon_j = 1\) for all \(j\). The lowest pair excitation corresponds\(^{21,22}\) to a single spin flip at the Fermi level \(\varepsilon_0 = 0\) and has an energy \(\Delta_2 = 2\Delta\). It also modifies the gap equation since now one of \(\varepsilon_j\) becomes negative, \(\varepsilon_0 = -1\). Because the number of states in the localization volume \(L_{loc}^3\) is finite, this modification results\(^{20,22}\) in a negative correction to the gap: \(\delta\Delta = -\delta L / 2\). Thus

\[
\Delta_2 = 2\Delta_0 - \delta\Delta = 2\Delta_0 - \frac{\lambda}{\nu_0 L_{loc}^2}
\]

where \(\Delta_0\) is the \(T = 0\) gap at large \(L_{loc}\), numerical coefficient \(c = 1\) for model \(4\) and \(c = \sim 1\) for model \(3\). Note that pair excitations with gap \(\Delta_2\) are spinless, whereas single-particle excitations (gap \(\Delta_1\) carry spin 1/2. Thus \(\Delta_1\) is the spin gap, while \(\Delta_2\) is the energy gap.

In the regime \(2\), the typical single-particle gap \(\Delta_1\) remains much larger than the gap for pair excitations \(\Delta_2\). This leads to the exclusion of single-particle excitations from the thermodynamics at \(T \ll \Delta_1\), which results in a modified mean-field result \(T_c / \Delta(T = 0) = 2[T_c / \Delta(T = 0)]_{BCS}\). The actual dependence of \(T_c\) on the localization length is not easy to find due to enhanced role of thermal fluctuations near the mobility edge.\(^{11,15}\)

We emphasize that \(\Delta(T = 0)\) does not characterize the spectral gap in the present situation. The most naturally measured (e.g. by tunneling conductance or optical conductivity experiments) spectral parameter is the
single-particle gap $\Delta_1$, which according to Eqs. (32) is much larger than $T_c$. An anomalously large ratio $\Delta_1/T_c$ leads to the insulating trend of the resistivity versus temperature behavior in the intermediate temperature range $T_c < T \leq \Delta_1$. This was observed in many strongly disordered superconductors and is especially well-known for underdoped cuprates.

The quantitative similarity between $R(T,B)$ behavior in InO$_x$ films and underdoped cuprates noticed in Ref. [26] (see also Ref. [27]) makes us believe the pseudogap in underdoped cuprates may have a similar origin: pairing of electrons on localized states. The important difference of the cuprates is the d-wave symmetry of the pairing. We plan to address this issue in future work. Suppression of single-particle density of states in the pseudogap regime can be observed by measuring the differential tunneling conductance which we expect to follow the universal IPR distribution $\mathcal{P}(M)$ studied in Ref. [18].

$$\frac{dI}{dV} \propto \left(\frac{dv}{d\varepsilon}\right)_{\varepsilon=eV} \propto \mathcal{P}(2eV\nu_0/\lambda)$$

(12)

As emphasized above, the generic features indicating a formation of the novel insulating state near superconductor-insulator transition (such as the resistivity maximum as a function of magnetic field or disorder) were observed in many different materials. However, the details may vary: in InO$_x$ thick (essentially 3D) films the resistivity above the transition has an activated behavior while in very thin (2D) films it follows an Efros-Shklovskii law. The theory developed in this Letter is applicable only to 3D systems but it seems likely that a similar physics leads to a weaker but observable effects in 2D films.

In conclusion, weak Anderson insulators with Cooper attraction are shown to possess hard insulating gap whose magnitude is determined by the IPR statistics near the mobility edge. Although this gap is of a superconducting origin, it does not lead to a coherence peak. In the ground-state of this insulator all electrons are paired on individual localized eigenfunctions. When the Fermi-level approaches the mobility edge, superconductive correlations develop between localized pairs. Key features of the predicted superconductive ground-state are an unusually large (compared to $T_c$) single-particle excitation gap (spin gap) and a pseudogapped regime at temperatures about $T_c$. These unusual features stem from the fractal nature of localized eigenstates near the mobility edge. We assumed that $\psi_0^d(r)$ of the relevant nearly-critical eigenfunctions have weak mutual correlations. If the correlations are in fact strong, the description of the insulating phase is not affected but the ratio $\Delta_1/\Delta \gg 1$ will be significantly reduced. Finally, our theory is based on a phenomenological assumption of an attractive sign of the diagonal coupling constant $\lambda > 0$. Another interesting situation is realized when $\lambda > 0$, but $\lambda < 0$. In this case we expect a formation of "effective magnetic impurities" and strong suppression of $T_c$. We plan to consider this situation separately.

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