Cooper problem in the vicinity of Anderson transition

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(November 29, 1999)

We study numerically the ground state properties of the Cooper problem in the three-dimensional Anderson model. It is shown that attractive interaction creates localized pairs in the metallic noninteracting phase. This localization is destroyed at sufficiently weak disorder. The phase diagram for the delocalization transition in the presence of disorder and interaction is determined.

PACS numbers: 74.20.-z, 72.15.Rn, 05.45.Mt

The pioneering experimental results for normal-state resistivity of high temperature superconductors demonstrated a striking correlation between the optimal doping with maximal $T_c$ in the superconducting phase and the Anderson metal-insulator transition (MIT) in the normal phase obtained in a strong pulsed magnetic field [1]. More recent experiments on the superconductor-insulator transition (SIT) in three dimensions (3D) [2,3], which were done in various materials at different dopings and magnetic fields, also reveal close correlation between these transitions even if it is possible that the normal state remains metallic in some materials [4,5]. These experimental results put forward the important theoretical problem of interaction effects in the vicinity of Anderson transition in 3D. However, the full understanding of this problem is very difficult since even the origin of the high-$T_c$ phase is not yet established completely. Due to that it would be interesting to understand the effects of interaction and disorder in a more simple model of generalized Cooper problem [6] of two quasiparticles above the frozen Fermi sea which interact via the attractive Hubbard interaction in the presence of disorder. In spite of apparent simplicity of this problem it is rather nontrivial. Indeed, even if the great progress has been reached recently in the investigation of localized one-particle eigenstate properties [7], the analytical expressions for the interaction induced matrix elements in the localized phase and in the MIT vicinity are still absent. Furthermore, the recent results for the problem of two interacting particles (TIP) in the localized phase demonstrated that the interaction effects for excited states can qualitatively change the eigenstate structure leading to the appearance of delocalization [7,8]. Due to that the investigation of the ground state properties of the above model in the vicinity of the Anderson transition in 3D represents an interesting unsolved problem which can shed light on the origin of SIT in the presence of disorder.

To investigate the above problem we study numerically the ground state properties of two particles with Hubbard on site attraction ($U < 0$) in 3D Anderson model at half filling. In this case the one particle eigenstates are determined by the Schrödinger equation

$$E_n \psi_n + V(\psi_{n-1} + \psi_{n+1}) = E\psi_n$$

where $n$ is the site index on the 3D lattice with periodic boundary conditions applied, $V$ is the nearest neighbour hopping and the random on-site energies $E_i$ are homogeneously distributed in the interval $[-W/2, W/2]$. It is well known that at half filling (the band center with $E = 0$) the MIT takes place at $W_c/V \approx 16.5$ with the insulating and metallic phases at $W > W_c$ and $W < W_c$ respectively (see e.g. [9,10]). To study this problem with interaction it is convenient to write its Hamiltonian in the

FIG. 1. Probability distributions for TIP in the ground state projected on $(x,y)$-plane: one particle probability $f_p$ for interaction $U = -4V$ (left column), interparticle distance probability $f_{pd}$ for $U = -4V$ (centrum column), $f_p$ for $U = 0$ (right column); the disorder strength is $W/W_c = 1.1$ (upper line), $W/W_c = 0.5$ (middle line), $W/W_c = 0.3$ (bottom line). All data are given for the same realisation of disorder for the system size $L = 16$ (see text for details). Upper line corresponds to the insulating noninteracting phase while two others are in the metallic one at $U = 0$. 

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basis of noninteracting eigenstates of the Anderson model that gives
\[(E_{m_1} + E_{m_2})\chi_{m_1, m_2} + U \sum_{m_1, m_2, m', m''} Q_{m_1, m_2, m', m''} \chi_{m', m''} = E\chi_{m_1, m_2}.\] (2)

Here \(\chi_{m_1, m_2}\) are eigenfunctions of the TIP problem written in one-particle eigenbasis \(\phi_m\) with eigenenergies \(E_m\). The transition matrix elements \(Q_{m_1, m_2, m', m''}\) are obtained by rewriting the Hubbard interaction in the noninteracting eigenbasis of model (1). The Fermi sea is introduced by restricting the sum in (2) to \(m_1, m_2 \geq 0\) with unperturbed energies \(E_{m_1, m_2} > E_F\). The value of the Fermi energy \(E_F \approx 0\) is determined by the filling factor \(\mu\) which is fixed at \(\mu = 1/2\). To have more close similarity with the Cooper problem we also introduce the high energy cut-off defined by the condition \(1 \leq m_1 + m_2 \leq M\). Such a rule gives an effective phonon frequency \(\omega_D \propto M/L^3\) where \(L\) is the linear lattice size. Since the frequency \(\omega_D\) should be independent of \(L\) we keep the ratio \(\alpha = L^3/M\) constant when varying \(L\). The majority of data are obtained for \(\alpha \approx 30\) but we checked that its variation by few times did not affect the results. Due to on-site nature of the Hubbard interaction only symmetric configurations are considered.

In fact the first studies of the model (2) with the frozen Fermi sea had been done by Imry [4] with the aim to analyze the delocalization effect of TIP in the proximity of Fermi level at finite particle density. This model was also studied numerically in [14] where it was shown that near \(E_F\) the interaction becomes effectively stronger comparing to the ergodic estimate used in [7,8]. However the above studies [4,14] were concentrated on the properties of excited states in the repulsive case \(U > 0\). On the contrary here we analyze the ground state properties for the attractive case. Since \(U < 0\), then even in the limit of large system size \(L\) the particles are always close to each other in the ground state that is qualitatively different from the case \(U > 0\). In this way the model (2) represents the generalized Cooper problem in the presence of disorder.

To study the characteristics of the ground state \(\chi^{(0)}_{m_1, m_2}\) we diagonalize numerically the Hamiltonian (3) and rewrite the eigenfunction in the original lattice basis \(|n\rangle\) with the help of relation between lattice basis and one particle eigenstates \(|n\rangle = \sum_m R_{n,m} \phi_m\). As the result of this procedure we determine the two particle probability distribution \(F(n_1, n_2)\) in the ground state (here \(n_{1,2}\) mark the positions of the two particles), from which the one particle probability \(f(n_1) = \sum_{n_2} F(n_1, n_2)\) and the probability of interparticle distance \(f_d(r) = \sum_{n_2} F(r + n_1, n_2)\) with \(r = n_1 - n_2\) are extracted. For graphical presentation these probabilities are projected on \((x, y)\)-plane that gives \(f_p(n_x, n_y) = \sum_{n_z} f(n_x, n_y, n_z)\) and \(f_{pd}(x, y)\) respectively. The typical examples of projected probability distributions \(f_p\) and \(f_{pd}\) for different values of disorder \(W\) are shown in Fig. 1. They clearly show that in the presence of interaction the ground state remains localized not only in the noninteracting localized phase \((W > W_c)\) but also in the phase delocalized at \(U = 0\) \((W < W_c)\). However the localized interacting phase abruptly disappears if disorder \(W\) becomes smaller than some critical value \(W_c(U) < W_c\). For \(W < W_c\) the ground state becomes delocalized over the whole lattice. At the same time the peaked structure of the interparticle distance distribution \(f_{pd}\) clearly shows that the particle dynamics remains correlated. In this sense we can say that the pairs exist for any strength of disorder but for \(W > W_c\) they are localized while for \(W < W_c\) they become delocalized. We assume that such a transition should correspond to the transition from insulating to superconducting phase in the many-body problem.

![FIG. 2. Dependence of IPR \(\xi\) on the rescaled disorder strength \(W/W_c\) for \(U = 0\) (\(\circ\)), \(U = -2V\) (\(\square\)), \(U = -4V\) (\(\triangle\)), \(U = -6V\) (\(\Delta\)) (empty/full symbols are for \(L = 10/L = 12\)). Insert shows the data for \(U = -4V\) at \(L = 8\) (\(\times\), 10 (\(\circ\), 12 (full diamond), 14 (\(\ast\)); \(\xi\) obtained in the Cooper approximation (see text) for \(U = -4V\), \(L = 14\) is shown by (\(\oplus\)). Statistical error-bars are smaller than symbol size. Lines are drawn to adapt an eye.](image-url)
mains finite and independent on size $L$ while in the delocalized phase it grows proportionally to the total number of sites $L^3$. To find the critical disorder strength $W_\text{c}$ we compare the relative change of $\xi$ with $L$ ($8 \leq L \leq 14$) with its relative change for the noninteracting case at the critical point $W = W_\text{c}$. Then $W_\text{c}(U)$ is defined as such a disorder at which the relative variation of $\xi$ at $|U| > 0$ becomes larger than in the case $U = 0$. We note that near the transition the change of $\xi$ with $W$ is so sharp that the delocalization border is not really sensitive to the choice of definition. We also checked that the change of $\omega_D$ does not affect significantly the border $W_\text{c}(U)$ \cite{3}. The phase diagram for SIT defined in the way described above is presented in Fig. 3. It shows that the interaction makes localization stronger so that the localized phase penetrates in the noninteracting metallic phase. However for sufficiently weak disorder delocalization takes over. Qualitatively we can say that the attraction creates a pair with a total mass ($m_1 + m_2$) twice larger than the one particle mass and due to that the critical disorder strength becomes twice smaller ($W_\text{c}/W_\text{c} \simeq 0.5$) since the effective hopping $V_{\text{eff}} \propto 1/m_p$. Of course this argument is not sufficient to explain the exact border $W_\text{c}(U)$ obtained numerically but it gives a reasonable estimate in the case of strong interaction. Further studies are required to explain the form of the border.

Another interesting physical characteristic is the coupling energy $\Delta$ of two particles in the presence of interaction. Its value is equal to $\Delta = 2E_F - E_g$ where $E_g$ is the ground state energy in the presence of interaction and $2E_F$ is equal to $E_g$ at $U = 0$. In the standard Cooper problem $\Delta > 0$ is related to the BCS gap and determines the correlation length of the pair. It is interesting to understand how $\Delta$ varies with the disorder strength $W$ at fixed interaction $U$. This dependence is presented in Fig. 4. It clearly shows that $\Delta$ grows significantly with the increase of $W$ at constant interaction $U$. We attribute the physical origin of this growth to the fact that at stronger disorder the rate of separation between particles becomes smaller that enhances enormously the interaction between them, hence $\Delta$, as it was discussed in \cite{3}. The dependence of $\Delta$ on $W$ is changed drastically near $W_\text{c}$ that is related to the delocalization transition.

On the same figure we compare the exact value of $\Delta$, found numerically in the model \cite{2}, with its value $\Delta_C$ obtained by the Cooper approximation (mean field value). In this approximation only the matrix elements $Q_{m_1, m_2, m_1', m_2'}$ with $m_1 = m_2$ and $m_1' = m_2'$ are kept in \cite{2} that corresponds to the original Cooper ansatz \cite{3}. The comparison shows that at weak disorder $\Delta_C$ is very close to exact $\Delta$ (see insert where dotted line coincides with full diamonds for $W/W_\text{c} < 0.35$) while when approaching the

![FIG. 3. Phase diagram for transition from localized (insulating I) to delocalized (superconducting S) phase in the ground state of the generalized Cooper problem \cite{1}. Vertical dashed line shows the Anderson transition in absence of interaction.](image)

![FIG. 4. Variation of the ground state coupling energy $\Delta$ in the model \cite{2} with the rescaled disorder strength $W/W_\text{c}$ for $L = 12$ and different interaction $U = -2V$ (full box), $U = -4V$ (full triangle), $U = -6V$ (full triangle); the open symbols are for the same $U$ values but in the Cooper approximation (see text). The vertical dashed line $W/W_\text{c} = 1$ marks the MIT at $U = 0$; the other vertical dashed line $W/W_\text{c} = 0.35$ marks approximately the SIT line from Fig. 3 for $|U| \geq 2$. Insert shows the case $U = -4V$ for $L = 10$ ($\circ$), $L = 12$ (full diamond), $L = 14$ ($\ast$); dotted line shows the Cooper approximation case with $U = -4V$ and $L = 12$ from the main figure; logarithm is decimal.](image)
Anderson transition and beyond it ($W/W_c > 0.35$) $\Delta_c$ becomes much smaller than $\Delta$. This leads to the conclusion that the nondiagonal matrix elements ($m_1 \neq m_2$ and $m_1' \neq m_2'$), neglected in the Cooper approximation, play an important role near MIT. This is also clear from Fig.1 according to which the localized states exist in the non-interacting metallic phase while according to the Cooper approximation pairs should be delocalized for $W < W_c$. Indeed, for example the graphical image as in Fig. 1 shows that for $U = -4V$, $W = 0.5W_c > W_s$ the probability $f_p$ obtained in the Cooper approximation from (2) is completely delocalized contrary to the real case in which the ground state is localized (Fig. 1). In addition to this case the average IPR within the Cooper approximation is much larger than its real value obtained without approximation (see insert in Fig. 2).

The data presented in the inserts of Fig. 2 and 3 clearly show that in the localized interacting phase $W > W_s$ the lattice size is sufficiently larger than the localization length and the values of $\xi$ and $\Delta$ correspond to the limit $L \to \infty$. At the same time for weak disorder $W/W_c < 0.2$ the asymptotic value of $\Delta$ is very small and very large values of $L$ are required to reach it. Such large $L$ are also desirable to see better the propagation of pairs with large size. The main increase of $\Delta$ takes place in the metallic noninteracting phase at $W_s < W < W_c$. However in this region the TIP pair remains localized due to interaction that does not allow to obtain a gain in the value of $\Delta \approx T_c$. It would be interesting to find some possibility to delocalize the pair in this region and to keep large $\Delta$ at the same time.

In conclusion, our numerical studies of the generalized Cooper problem in the presence of disorder show that in the ground state the attractive interaction leads to localization of pairs inside noninteracting metallic phase, contrary to the Cooper ansatz. This localization however disappears at sufficiently weak disorder. The phase diagram for the transition to delocalized states is determined as a function of disorder and interaction.

We thank V.V.Flambaum, K.Frahm and O.P.Sushkov for stimulating discussions, and the IDRIS in Orsay and the CICT in Toulouse for access to their supercomputers.

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