Cooper problem in the vicinity of the Anderson transition

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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.

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] Namely, the MIT in strong magnetic field takes place at such a doping for which T_c is maximal at zero magnetic field. More recent experiments on the superconductor-insulator transition (SIT) in three dimensions (3D),[2–4] 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.[2,4] 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[5] 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,[6] 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.[7–10] 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

$$E_{\mathbf{n}}\psi_{\mathbf{n}}+V(\psi_{\mathbf{n-1}}+\psi_{\mathbf{n+1}})=E\psi_{\mathbf{n}}, \tag{1}$$

where $\mathbf{n}$ is the site index on the 3D lattice with periodic boundary conditions applied, V is the nearest-neighbor 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., Refs. 11,12). To study this problem with interaction it is convenient to write its Hamiltonian in the basis of noninteracting eigenstates of the Anderson model that gives

$$(E_{m_1}+E_{m_2})\chi_{m_1,m_2}+U\sum_{m_1',m_2'} Q_{m_1,m_2,m_1',m_2'}\chi_{m_1',m_2'} = E\chi_{m_1,m_2}. \tag{2}$$

Here χ_{m_1,m_2} are eigenfunctions of the TIP problem written in one-particle eigenbasis ϕ_m with eigenenergies E_m. The transition matrix elements $Q_{m_1,m_2,m_1',m_2'}$ are obtained by rewriting the Hubbard interaction in the noninteracting eigenbasis of model (1). The Fermi sea is introduced by restricting the sum in Eq. (2) to $m_{1,2}'>0$ with unperturbed energies $E_{m_{1,2}'}>E_F$. The value of the Fermi energy $E_F\approx 0$ is determined by the filling factor μ which is fixed at $\mu=1/2$. To have more close similarity with the Cooper problem we also introduce the high energy cutoff defined by the condition $1\leqslant m_1'+m_2'\leqslant M$. Such a rule gives an effective phonon frequency $\omega_D\propto M/L^3$ where L is the linear lattice size. Since the frequency ω_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 $\alpha\approx 30$ (Ref. 13) 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[8] 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 Ref. 14 where it was shown that near E_F the interaction becomes effectively stronger comparing to the ergodic estimate used in Refs. 7,8. However the above studies[8,14] 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

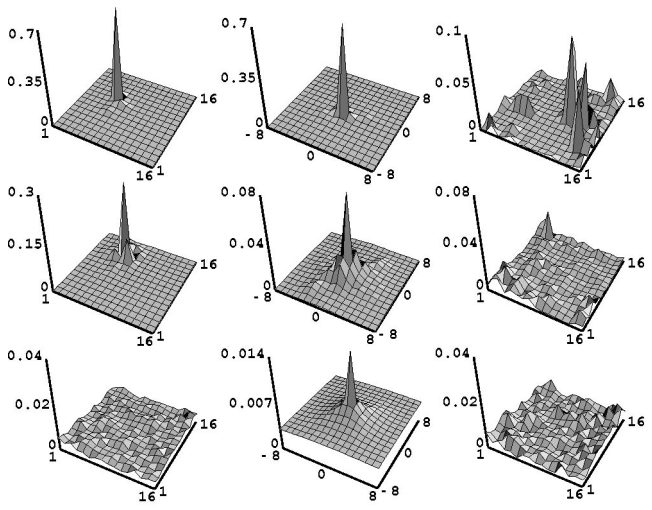

FIG. 1. Probability distributions for TIP in the ground state projected on the (x,y) plane: one particle probability f_p for interaction $U=-4V$ (left column), interparticle distance probability f_{pd} for $U=-4V$ (centrum column), f_p for $U=0$ (right column); the disorder strength is $W/W_c=1.1$ (upper line), $W/W_c=0.5$ (middle line), $W/W_c=0.3$ (bottom line). All data are given for the same realization 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 $U=0$.

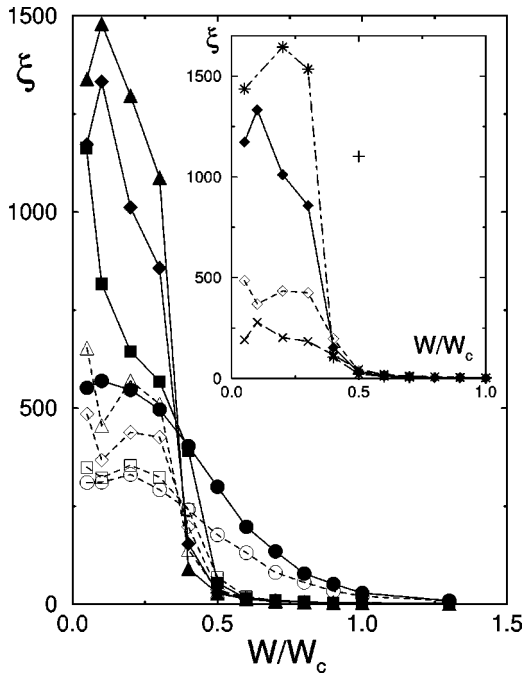

FIG. 2. Dependence of IPR ξ on the rescaled disorder strength W/W_c for $U=0$ ($\bigcirc$), $U=-2V$ ($\square$), $U=-4V$ ($\diamond$), $U=-6V$ ($\triangle$) (empty/full symbols are for $L=10/L=12$). The inset shows the data for $U=-4V$ at $L=8$ ($\times$), 10 ($\diamond$), 12 (full diamond), 14 (*); ξ obtained in the Cooper approximation (see text) for $U=-4V$, $L=14$ is shown by (+). Statistical error bars are smaller than symbol size. Lines are drawn to adapt an eye.

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 (2) and rewrite the eigenfunction in the original lattice basis $|\mathbf{n}\rangle$ with the help of relation between lattice basis and one particle eigenstates $|\mathbf{n}\rangle=\Sigma_m R_{\mathbf{n},m}\phi_m$. As the result of this procedure we determine the two particle probability distribution $F(\mathbf{n}_1,\mathbf{n}_2)$ in the ground state (here $\mathbf{n}_{1,2}$ mark the positions of the two particles), from which the one particle probability $f(\mathbf{n}_1)=\Sigma_{\mathbf{n}_2}F(\mathbf{n}_1,\mathbf{n}_2)$ and the probability of interparticle distance $f_d(\mathbf{r})=\Sigma_{\mathbf{n}_2}F(\mathbf{r}+\mathbf{n}_2,\mathbf{n}_2)$ with $\mathbf{r}=\mathbf{n}_1-\mathbf{n}_2$ are extracted. For graphical presentation these probabilities are projected on (x,y) plane that gives $f_p(n_x,n_y)=\Sigma_{n_z}f(n_x,n_y,n_z)$ 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 $W_s(U)<W_c$. For $W<W_s$ 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 $W>W_s$ they are localized while for $W<W_s$ they become delocalized. We assume that such a transition should correspond to the transition from insulating to superconducting phase in the many-body problem.

To analyze this transition in a more quantitative way we determine the inverse participating ratio (IPR) ξ for one particle probability: $1/\xi=\langle\Sigma_{\mathbf{n}}f^2(\mathbf{n})\rangle$, where brackets mark the averaging over 100 disorder realizations. Physically, ξ counts the number of sites occupied by one particle in the ground state. Its variation with system size L is shown in Fig. 2 for different strength of interaction and disorder. This figure shows that in the localized interacting phase $W>W_s(U)$ the ξ value remains 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_s we compare the relative change of ξ with L ($8\leqslant L\leqslant 14$) with its relative change for the noninteracting case at the critical point $W=W_c$. Then $W_s(U)$ is defined as such a disorder at which the relative variation of ξ at $|U|>0$ becomes larger than in the case $U=0$. We note that near the transition the change of ξ 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 ω_D does not affect significantly the border $W_s(U)$.[16] 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 (insulating) phase penetrates in the noninteracting (normal) metallic phase. However, for sufficiently weak disorder delocalization takes over. This is in agreement with the Anderson theorem according to which a weak disorder in metallic phase does not affect superconductivity.[15] Qualitatively we can say that the attraction creates a pair with a total mass (m_p) twice larger than the one particle mass and due to that the critical disorder strength for localization becomes twice smaller ($W_s/W_c\simeq 0.5$) since the effective hopping $V_{eff}\propto 1/m_p$. Of course

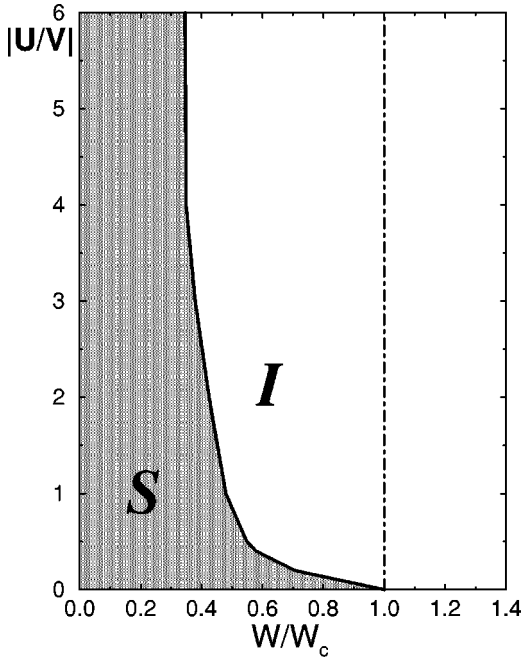

FIG. 3. Phase diagram for transition from localized (insulating I) to delocalized (superconducting S) phase in the ground state of the generalized Cooper problem (2). Vertical dashed line shows the Anderson transition in absence of interaction.

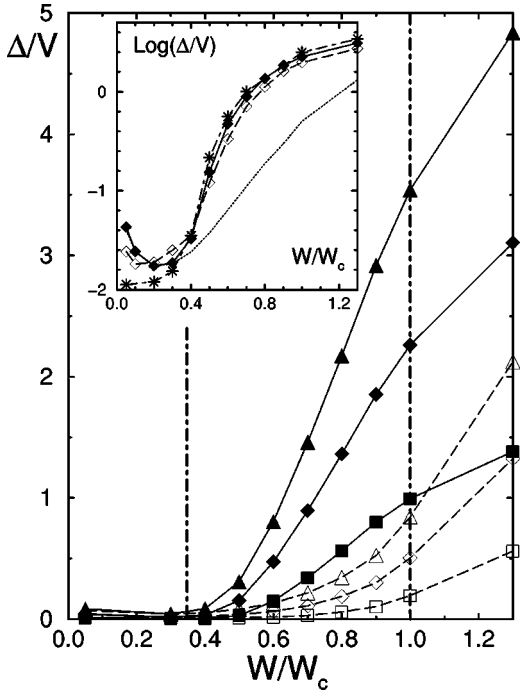

FIG. 4. Variation of the ground state coupling energy Δ in the model (2) with the rescaled disorder strength W/W_c for $L=12$ and different interaction $U=-2V$ (full box), $U=-4V$ (full diamond), $U=-6V$ (full triangle); the open symbols are for the same U values but in the Cooper approximation (see text). The vertical dashed line $W/W_c=1$ marks the MIT at $U=0$; the other vertical dashed line $W/W_c=0.35$ marks approximately the SIT line from Fig. 3 for $|U|\geqslant 2$. The insert shows the case $U=-4V$ for $L=10$ ($\diamond$), $L=12$ (full diamond), $L=14$ (*); the dotted line shows the Cooper approximation case with $U=-4V$ and $L=12$ from the main figure; logarithm is decimal.

this argument is not sufficient to explain the exact border $W_s(U)$ 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 Δ 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.[17] It is interesting to understand how Δ varies with the disorder strength W at fixed interaction U. This dependence is presented in Fig. 4. It clearly shows that Δ 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 Δ, as it was discussed in Ref. 14. The dependence of Δ on W is changed drastically near W_s that is related to the delocalization transition.

On the same figure we compare the exact value of Δ, found numerically in the model (2), with its value Δ_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 Eq. (2) that corresponds to the original Cooper ansatz.[5] The comparison shows that at weak disorder Δ_C is very close to exact Δ (see the inset where dotted line coincides with full diamonds for $W/W_c<0.35$) while when approaching the Anderson transition and beyond it ($W/W_c>0.35$) Δ_C becomes much smaller than Δ. 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 noninteracting 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 Eq. (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 inset in Fig. 2).

The data presented in the insets of Figs. 2 and 4 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 ξ and Δ correspond to the limit $L\to\infty$.[18] Indeed, for example for $W=0.4W_c$, $U=-4V$ the value of Δ varies only by 6% around the average $\Delta=0.035V$ when L changes from 10 to 16. On the contrary, the first order correction in U to Δ, computed over noninteracting delocalized eigenstates, drops 4 times ($\propto 1/L^3$). This fact, in combination with other data in the inset of Fig. 4 and a peaked probability distribution in interparticle distance $f_d(\mathbf{r})$ in the middle column of Fig. 1, clearly shows the formation of localized pairs in the noninteracting metallic phase. At the same time for weak disorder $W/W_c<0.2$ the asymptotic value of Δ becomes 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. We note that Δ increases strongly 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 $\Delta \simeq T_c$. It would be interesting to find some possibility to delocalize the pair in this region and to keep large Δ at the same time.

In conclusion, our numerical studies of the generalized Cooper problem show that at sufficiently strong disorder, at which, however, the noninteracting particles are still delocalized (noninteracting metallic phase), the attractive interaction with a strength larger than some critical value leads to localization of pairs in the ground state, contrary to the Cooper ansatz. This localization, however, disappears at sufficiently weak disorder in agreement with the Anderson theorem.[15] The phase diagram for the transition to delocalized states is determined as a function of disorder and interaction. The appearance of SIT in the normal (noninteracting particles) metallic phase is in a qualitative agreement with the experiments[4] which show that the ''ground state'' of the normal state of YBCO is metallic. Indeed, an applied magnetic field effectively decreases the attraction U between quasiparticles and also eliminates the supraconducting gap that should drive the system to the normal (noninteracting particles) metallic phase. This is in a qualitative agreement with our results according to which the decrease in interaction strength U can lead to a more delocalized state. However, further studies of the generalized Cooper problem with a magnetic field are required for a quantitative analysis of magnetic field effects.

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*URL: http://w3-phystheo.ups-tlse.fr/~dima

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[16] For example $W_s/W_c \approx 0.35/0.36$ for $\alpha = 30/15$ at $U = -4V$.

[17] For $U < 0$ the value of Δ is always positive, however, one should also show that Δ is independent of system size L to attribute to it the usual meaning of coupling energy. The data in the inset of Fig. 4 clearly show that this is the case unless the size of the pair becomes comparable with the lattice size available for our numerical simulations.

[18] We checked that for $W > W_s$, e.g., $W = 12V$, $U = -4V$, the excited states with $E - 2E_F < 0$ also remain localized, J. Lages and D. L. Shepelyansky (unpublished).