Phase of bi-particle localized states for the Cooper problem in two-dimensional disordered systems

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The Cooper problem is studied numerically for the Anderson model with disorder in two-dimensions. It is shown that the attractive Hubbard interaction creates a phase of bi-particle localized states in the regime where non-interacting states are delocalized. This phase cannot be obtained in the mean-field approximation and the pair coupling energy is strongly enhanced in this regime. The effects of magnetic field are studied and it is shown that under certain conditions they lead to delocalization.

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I. INTRODUCTION

Recently a great deal of attention has been attracted to investigation of superconductor-insulator transition (SIT) in systems with disorder. Various approaches are used to study this problem including analytical theoretical methods [1,2], intensive numerical simulations of many-body quantum systems with quantum Monte Carlo methods [3,4], as well as mean field numerical simulations [5–7]. These theoretical studies are stimulated by challenging experiments on SIT in disordered films [8,9] and restricted to systems of quite moderate size (for example lattices of 8x8 sites in [4]). Indeed the direct diagonalization methods are restricted to relatively small system size since the Hilbert space grows exponentially with the number of particles [14,15]. The quantum Monte Carlo methods are not so sensitive to a huge size of the Hilbert space but still they are restricted to systems of quite moderate size (for example lattices of 8x8 sites in [4]).

In the view of above numerical difficulties it is natural to develop the approach introduced by Cooper [10] and to study the problem of two particles with attractive interaction near the frozen Fermi sea in the presence of disorder. Even if the original Cooper problem of two particles without disorder does not reproduce exactly the BCS theory of many-body problem it nevertheless captures the essential physical properties of the system and gives the appearance of coupled states with a qualitatively correct coupling energy and correlation length. Without disorder the Cooper problem can be solved exactly. However in presence of disorder the situation becomes more complicated even for only two interacting particles (TIP). Indeed, for relatively strong disorder even the matrix elements of interaction between non-interacting eigenstates can not be obtained analytically and due to that the problem should be studied numerically. The first numerical studies of the Cooper problem in the presence of disorder were done in [17] for two particles with attractive Hubbard interaction in the three-dimensional Anderson model. These studies showed that the interaction can lead to localization of pairs in the non-interacting metallic phase. This result is qualitatively different from the mean field solution of the Cooper problem in the presence of disorder (Cooper ansatz) which gives delocalized pairs for the same parameters. This shows that the non-diagonal interaction induced matrix elements play an important role and lead to new physical effects which are not captured by the mean field approximation.

In this paper we study the Cooper problem on a two-dimensional lattice with disorder described by the Anderson model. Our numerical studies show that near the Fermi level the attractive Hubbard interaction between two particles creates localized pairs in the regime where non-interacting eigenstates are well delocalized (extended). The coupling energy of these pairs is much larger than the coupling energy given by the mean field solution (Cooper ansatz). Therefore energetically it is more favorable to have an insulator with localized pairs instead of usual weakly coupled delocalized Cooper pairs. This result indicates the appearance of a new phase of bi-particle localized states (BLS phase) which appears in the regime when non-interacting states are extended (metal-
particle eigenstates are determined by the Hamiltonian dimensional Anderson model. In this model the one-particles in the presence of disorder we use the two-and disorder are analyzed in Section 3. The discussion the ground state properties in the presence of interaction and disorder are discussed in Section 2. The effects of perpendicular magnetic field on the ground state properties in the presence of interaction and disorder are analyzed in Section 3. The discussion of the results is presented in the last Section.

II. GROUND STATE PROPERTIES WITHOUT MAGNETIC FIELD

To study the Cooper problem of two interacting particles in the presence of disorder we use the two-dimensional Anderson model. In this model the one-particle eigenstates are determined by the Hamiltonian

$$H_1 = \sum_n E_n |n\rangle \langle n| + V \sum_{\langle n,m \rangle} |n\rangle \langle m|$$

(1)

where $n$ and $m$ are index vectors on the two-dimensional square lattice with periodic boundary conditions, $V$ is the nearest neighbor hopping term and the random on-site energies $E_n$ are homogeneously distributed in the energy interval $[-W, W]$, where $W$ is the disorder strength. This one-particle model has been extensively studied by different authors, see for example [19]. For the two-particle problem on this two-dimensional lattice we consider on-site attractive Hubbard interaction between particles of strength $U < 0$. We consider the particles in the singlet state with zero total spin so that the spatial wavefunction is symmetric with respect to particle permutation (interaction is absent in the triplet state).

To investigate the effects of interaction between particles near the Fermi level we generalize the Cooper approach for the case with disorder. To do that we rewrite the TIP Hamiltonian in the basis of one-particle eigenstates of the Hamiltonian [1]. In this basis the Schrödinger equation for TIP reads

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

(2)

Here $E_m$ are the one-particle eigenenergies corresponding to the one-particle eigenstates $|\phi_m\rangle$ and $\chi_{m_1,m_2}$ are the components of the TIP eigenstate in the non-interacting eigenbasis $|\phi_{m_1}, \phi_{m_2}\rangle$. The matrix elements $UQ_{m_1,m_2,m_1',m_2'}$ gives the interaction induced transitions between non-interacting eigenstates $|\phi_{m_1}, \phi_{m_2}\rangle$ and $|\phi_{m_1'}, \phi_{m_2'}\rangle$. These matrix elements are obtained by rewriting the Hubbard interaction in the non-interactive eigenbasis of model [1]. In the analogy with the original Cooper problem [11] the summation in (3) is done over the states above the Fermi level with eigenenergies $E_{m_1,m_2} > E_F$ with $m_{1,2} > 0$. The Fermi energy $E_F \approx 0$ is determined by a fixed filling factor $\nu = 1/2$. To keep the similarity with the Cooper problem we restrict the summation on $m_{1,2}$ by the condition $1 < m_1 + m_2 \leq M$. In this way the cut-off with $M$ unperturbed orbitals introduces an effective phonon frequency $\omega_D \propto M/L^2 = 1/\alpha$ where $L$ is the linear system size. When varying $L$ we

![FIG. 1. Ground state probability distributions of two interacting particles for the Cooper problem with disorder on a lattice of linear size $L = 40$. The cases (a,b) show one particle probability distribution $f(n)$ in absence of interaction ($U = 0V$) for the disorder strength $W = 2V$ (a) and $W = 5V$ (b). All other cases are obtained for the Hubbard interaction $U = -2V$. The cases (c,d) show the one-particle probability $f(n)$ (c) and the interparticle distance probability $f_d(r)$ (d) for $W = 2V$. The same probabilities are shown in cases (e,f) for $W = 5V$ ($f(n)$ for (e) and $f_d(r)$ for (f)). The cases (g,h) present the probabilities for the same $W = 5V$ as in cases (e,f) however here the ground state is obtained in the mean field approximation of the Cooper ansatz. All data are given for the same realization of disorder.](image)
keep $\alpha$ fixed so that the phonon frequency is independent of system size. All the data in this work are obtained with $\alpha = 15$ but we also checked that the results are not sensitive to the change of $\alpha$. We note that a similar TIP model was considered for the problem of two repulsive quasiparticles near the Fermi level in $[20,21]$. However, there the studies were mainly addressed to the properties of excited states while here we will investigate only the properties of the ground state in the case of an attractive interaction. We also note that the attractive case in one-dimension was discussed in $[22,23]$.

To determine the characteristics of the ground state of the generalized Cooper problem $[2]$ we solved numerically the Schrödinger equation. After that we rewrite the obtained ground state in the original lattice basis with the help of the relation between lattice basis and one-particle eigenstates $|n\rangle = \sum_{m} R_{n,m} |\phi_{m}\rangle$. As a result of this procedure we obtain the two-particle probability distribution $F(n_1, n_2)$ from which we extract the one-particle probability $f(n) = \sum_{n_2} F(n_1, n_2)$ and the probability of interparticle distance $f_d(r) = \sum_{n_2} F(r + n_2, n_2)$ with $r = n_1 - n_2$.

Typical examples of such probability distributions are presented in Fig. 1. Without interaction, at given disorder strength $W = 2V$ and $W = 5V$ both particles are delocalized on the lattice of given size $L = 40$. In presence of interaction $U = -2V$ the ground state remains delocalized for $W = 2V$ and the probability distribution is rather similar to the case of $U = 0$ (compare Figs.1a and 1c). On the contrary for $W = 5V$ interaction completely changes the ground state properties leading to a clear localization of both particles near each other (compare Figs.1b and 1e). The wavefunction is localized in a rather compact way and the finite size of the lattice definitely does not affect this localization. Fig.1f shows that in this localized state the particles remain correlated being close to each other. This bi-particle localized ground state is obtained by exact diagonalization of $[3]$ where all non-diagonal interaction induced matrix elements are taken into account. It is interesting to compare this solution with the mean field approximation (Cooper ansatz) in which only diagonal terms are taken into account. Within the Cooper ansatz the particles occupy the same non-interacting orbitals and only matrix elements $Q_{m_1,m_2,n_1,n_2}$ with $m_1 = m_2$ and $n_1 = n_2$ are kept in $[3]$. The ground state obtained from the Cooper ansatz is shown in Figs.1g and 1h and is clearly delocalized contrarily to the strongly localized ground state obtained from exact diagonalization of $[2]$ and shown in Figs.1e and 1f. In fact the ground state from the Cooper ansatz is more close to delocalized non-interacting eigenstate in Fig.1b than to the real eigenstate in Fig.1e in the presence of interaction. The results of Fig.1 definitely show that the attractive interaction leads to localization of pairs in the regime when non-interacting states are delocalized. This localization is not captured by the Cooper ansatz which neglects non-diagonal matrix elements and due to that misses the essential physical effect.

FIG. 2. Dependence of the inverse participation ratio $\xi$ of the TIP ground state on the disorder $W/V$. The full lines with full symbols correspond to an interaction strength $U = -4V$, the dashed ones with open symbols to $U = -2V$ and the dot-dashed ones to $U = 0V$ (+, x, *). Different symbols correspond to different linear size of the lattice $L = 20$ (◦, +), $L = 30$ (♦, ×), and $L = 40$ (∆, *).

In order to study the ground state properties of our model in a more quantitative way it is convenient to compute the inverse participation ratio (IPR) $\xi$ defined as $\xi = \langle \sum_{n} f^2(n) \rangle$ where the brackets mark the averaging over $N_D$ disorder realizations (typically $N_D = 100$). Physically, $\xi$ gives the number of lattice sites occupied by one particle in the TIP ground state. The dependence of the IPR $\xi$ on the disorder strength $W$ is shown in Fig.2 for different strength of interaction $U$ and different system sizes $L$. In the absence of interaction, for finite system sizes used in our numerical simulations ($L \leq 40$), the ground state is delocalized for disorder $W \leq 5V$ and it becomes localized for $W > 5V$. On the contrary in the presence of interaction the TIP ground state becomes delocalized for $W > W_c \approx 2V$ at $U = -4V$ and for $W > W_c \approx 3V$ at $U = -2V$. Indeed for $W < W_c$ the IPR $\xi$ starts to grow significantly with the increase of the system size $L$ that corresponds to pair delocalization. The decrease of the $W_c$ value induced by the attractive interaction shows that the attraction leads to localization of pairs inside the non-interacting delocalized phase. This effect is absent in the mean field approximation where the ground state remains well delocalized (compare Figs. 1e and 1g). This phenomenon is similar to the situation in three-dimensional Anderson model for which the localiza-
The difference between exact diagonalization of the TIP Hamiltonian (2) and the mean field solution given by the Cooper ansatz is also clearly seen in the coupling energy of pair $\Delta = E_q(U = 0) - E_q(U)$. Here $E_q$ is the TIP ground state energy in presence of interaction $U$. For $U = 0$ we have $E_q(U = 0) = 2E_F$. The dependence of $\Delta$ on the disorder strength $W$ is shown in Fig.4 for $U = -2V$. The linear lattice size is $L = 20$ ($\circ$) and $L = 40$ ($\triangle$); data are obtained by exact diagonalization of TIP model (solid lines, full symbols) and by mean field approximation from the Cooper ansatz (dashed lines, empty symbols).

The physical reason for the increase of $\Delta$ comparing to the mean field value is related to localization: the pairs are localized and particles remains closer to each other that effectively increases the coupling strength between them [24]. On the contrary for $W < W_c$ when the pairs are delocalized the exact solution gives the value of $\Delta$ treated exactly (up to statistical errors) by the quantum Monte Carlo method. The presence of other fermions can renormalize effective strength of interaction between two particles. Also it can change the effective strength of disorder for fermions near the Fermi level. The comparison between the two figures shows that the TIP approach captures the qualitative physical properties of the system but quantitatively it gives different values. In a sense this situation is similar to the comparison between the Cooper approximation and the BCS theory.
ues of $\Delta$ which are close to the mean field value. This is in agreement with the Anderson theorem according to which mean field remains valid in the regime with weak disorder.

The fact that for TIP the BLS phase is energetically more favorable than the mean field solution indicates that also at finite particle density the BLS phase will be more favorable. This indication is in agreement with the quantum Monte Carlo computations presented in [18]. It is also possible to give another argument in the favor of BLS phase. Suppose that the filling factor $\nu$ is close to the critical value $\nu_c$ at the mobility edge of non-interacting particles (but $\nu > \nu_c$). Then it is natural that all particles below the mobility edge are localized. Then the density of interacting pairs above $\nu_c$ is proportional to $|\nu - \nu_c|$ and is relatively low for $|\nu - \nu_c| \ll \nu$. In this regime the pairs above $\nu_c$ are well separated and the TIP approximation we discuss in this paper should be rather reasonable. Of course on the next step the residual interaction between pairs should be taken into account [26]. In this picture it is clear that the BLS phase is energetically more favorable comparing to the delocalized mean field solution.

### III. GROUND STATE PROPERTIES WITH MAGNETIC FIELD

It is interesting to understand how the TIP properties in the BLS phase are affected by a magnetic field $\mathbf{B}$ perpendicular to the two-dimensional lattice. In this case the one-particle Hamiltonian takes the form

$$H_1 = \sum_n E_n \langle n | | n \rangle + V \sum_n \langle T(n) + T^\ast(n) \rangle$$

where $T(n)$ and $T^\ast(n)$ are the translation operators from site $n$ to its nearest neighbours.

$$T(n) = T_{M_x}(n) | n \rangle \langle n + e_x | + T_{M_y}(n) | n \rangle \langle n + e_y |.$$  \hspace{1cm} (4)

Here $e_x$ and $e_y$ are the unitary vectors on the two dimensional lattice and

$$T_{M_{x(y)}}(n) = \exp \left( -\frac{iq}{\hbar c} \int_{\Gamma_{x(y)}(n)} A \cdot d\mathbf{n}' \right)$$ \hspace{1cm} (5)

are the magnetic translation operators along paths $\Gamma_x(n) = (n \rightarrow n + e_x)$ and $\Gamma_y(n) = (n \rightarrow n + e_y)$. For convenience we choose the Landau’s gauge for the magnetic field $\mathbf{A} = -ny \mathbf{B} \mathbf{e}_x$. The magnetic translation operators are then determined as $T_{M_x} = \exp(2\pi i \gamma y u_n)$ and $T_{M_y} = 1$ with $\gamma = \frac{\pi q}{\hbar c}$. Due to the periodic boundary conditions the effective topology of the two-dimensional lattice is that of a torus with a transversal and a longitudinal radius $R_l = R_t = L$. This topology implies flux quantization on the lattice so that $\gamma = \frac{n\phi}{\Phi_0}$ with $m \in [0, L - 1]$. Then the one-particle Hamiltonian \(^3\) can be explicitly written as

$$H_1 = \sum_n E_n | n \rangle \langle n | + \sum_n \left( e^{i \pi \gamma y u_n} | n + e_x \rangle \langle n | + | n + e_y \rangle \langle n | \right) + \sum_n \left( e^{-i \pi \gamma y u_n} | n + e_x \rangle \langle n | + | n + e_y \rangle \langle n | \right).$$  \hspace{1cm} (6)

\FIG. 5. Ground state probability distributions of two interacting particles in a lattice of linear size $L = 40$, with disorder strength $W = 3V$, and interaction strength $U = -2V$; the left column shows the probability distribution $f(n)$ and the right one the interparticle probability distribution $f_d(r)$. The different rows present the TIP ground state for different value of the magnetic flux $\gamma$: top row $\gamma = 0$, middle row $\gamma = \frac{\pi}{20}$, and bottom row $\gamma = \frac{\pi}{10}$.

We study now the ground state of the TIP Hamiltonian constructed with this new one-particle Hamiltonian $H_1$ \(^3\). This Hamiltonian is written in the preferential basis of non-interacting eigenstates of \(^3\) that leads to the Schrödinger equation of the form \(^3\). As in the case with $\mathbf{B} = 0$ we use the probability distributions $f(n)$, $f_d(r)$ and the IPR $\xi$ to depict the ground state properties of the TIP problem in presence of a magnetic field. Thus Fig.\(^3\) represents the TIP probability distributions for a system of linear size $L = 40$ and fixed disorder and interaction.
strengths \((W = 3V, U = -2V)\). The data are shown for different magnetic flux ratios \(\gamma = 0, \gamma = \frac{2}{40}\), and \(\gamma = \frac{5}{40}\). At \(\gamma = 0\) the one particle probability is well localized by interaction (first row of Fig.5). However, with the increase of magnetic flux \(\gamma\) the localization is destroyed. The data of Fig.5 suggest that there exists a critical magnetic flux \(\gamma_c\) below which the TIP pairs remain localized \((\gamma < \gamma_c)\), middle row of Fig.5 and above which pairs become totally delocalized \((\gamma > \gamma_c)\), bottom row of Fig.5). At the same time for \(\gamma > \gamma_c\) the interparticle distance probability distribution \(f_d(r)\) is less peaked. Hence for \(\gamma > \gamma_c\) the size of the pair is significantly increased.

The ground state properties can be studied in a more quantitative way with the help of the IPR \(\xi\) defined above. Fig.6 represents the dependence of \(\xi\) on the disorder strength \(W/V\) for a fixed interaction \(U = -2V\). Data are shown for different values of magnetic flux \(\gamma\). They clearly show that the introduction of magnetic field leads to an increase of \(\xi\) at a fixed value of \(W\). Thus the magnetic field enhances the delocalization of particles for \(\gamma > \gamma_c(U)\) and \(W < W_c(U)\). On the contrary for \(\gamma < \gamma_c(U)\) and \(W > W_c(U)\) the variation of \(\xi\) with lattice size \(L\) is weak and usually here there is a small decrease of \(\xi\) with increase of \(L\) (see Fig.6). The delocalization transition can be determined as the point where \(\xi\) is independent of the lattice size (crossing point). An approximate phase diagram in the plane \((W, \gamma)\) obtained in this way is shown in the inset of Fig.6. With the increase of interaction the localized phase penetrates deeper in the region of weak disorder. The fact that a magnetic field can delocalize pairs inside the BLS phase is also illustrated in Fig.6 where the IPR \(\xi\) is enormously increased by the magnetic flux. This result is in agreement with a
general fact known for non-interacting particles that the localization length is increased by a magnetic field \[ \frac{\gamma}{\Delta} \]. While the delocalization induced by a magnetic field is clearly illustrated by the Figs. \[ \text{Fig.} \] and \[ \text{Fig.} \] it is rather difficult to determine numerically the properties of pairs in the delocalized phase. In this phase an effective pair size becomes too large to investigate it numerically. The question if the superconductivity survives or if a magnetic field drives the system to a metallic regime is difficult to answer in the frame of our numerical approach.

For a better understanding of both localized and delocalized phases we studied the dependence of the pair coupling energy \( \Delta \) on the strength of magnetic field. In the standard Cooper problem \( \Delta \) is related to the BCS gap and determines the Cooper pair size \( l_{\text{pair}} \propto 1/\Delta \). Fig. \[ \text{Fig.} \] shows the dependence of \( \Delta \) on the magnetic field for different lattice sizes and for the case \( U = -2V \) and \( W = 3V \), already used in the Fig. \[ \text{Fig.} \]. In the localized regime with \( \gamma < \gamma_c \approx 0.04 \) the value of \( \Delta \) varies weakly with the growth of \( L \). In contrast, for \( \gamma > \gamma_c \) its value decreases in 2 - 3 times. This can be considered as an indication that the superconductivity is significantly suppressed by magnetic field for \( \gamma > \gamma_c \). However, a significant increase of \( L \) is required to investigate the properties of pairs in the delocalized regime.

### IV. CONCLUSION

The present studies show that in the presence of disorder the attractive Hubbard interaction leads to localization of pairs and appearance of phase with bi-particle localized states which is located inside the non-interacting metallic regime. This BLS phase cannot be obtained in the mean-field approximation. It is shown that it can be destroyed by the introduction of a magnetic field which drives the system to delocalization. In the BLS phase the pair coupling energy is much larger than the value obtained in the mean-field approximation. This indicates that the BLS phase is energetically more preferable comparing to the mean-field solution. The results obtained for two particles (one pair) are in qualitative agreement with the recent results obtained with the quantum Monte Carlo in \[ \text{Fig.} \].

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[1] A. Larkin, Ann. Phys.(Leipzig) \textbf{8}, 785 (1999).

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