Delocalization of two-particle ring near the Fermi level of 2d Anderson model

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We study analytically and numerically the problem of two particles with a long range attractive interaction on a two-dimensional (2d) lattice with disorder. It is shown that below some critical disorder the interaction creates delocalized coupled states near the Fermi level. These states appear inside well localized noninteracting phase and have a form of two-particle ring which diffusively propagates over the lattice.

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Recently a great deal of attention has been attracted to the problem of interaction effects in disordered systems with Anderson localization [1,2]. From the theoretical point of view the problem is rather nontrivial. Indeed, even if a great progress has been reached in the theoretical investigation of the properties of localized eigenstates [3] still the analytical expressions for interaction matrix elements between localized states are lacking. In spite of these theoretical difficulties it has been shown recently that a repulsive or attractive interaction between particles can destroy localization and lead to a propagation of pairs in the noninteracting localized phase. This two interacting particles (TIP) effect has been studied recently by different groups [4,5] and it has been understood that the delocalization of TIP pairs is related to the enhancement of interaction in systems with complex, chaotic eigenstates. Such an enhancement had been already known for parity violation induced by the weak interaction near the Fermi level [6,7] where the interaction is typically increased by a factor of thousand. However, since there the two-body interaction is really weak the final result still remains small. On the contrary, for TIP pairs in the localized phase the enhancement of interaction qualitatively changes the dynamics leading to a coherent propagation of TIP on a distance $l_c$ being much larger than the pair size and one-particle localization length $l_1$. The enhancement factor $\kappa$ is determined by the density of two-particle states $\rho_2$, coupled by interaction, and the interaction induced transition rate $\Gamma_2$ between noninteracting eigenstates, so that $\kappa = \Gamma_2/\rho_2$. At $\kappa \sim 1$ the interaction matrix element becomes comparable with two-particle level spacing and the Anderson localization starts to be destroyed by interaction. For excited states the TIP density $\rho_2$ is significantly larger than the one-particle density $\rho$ and the delocalization can be reached for relatively weak interaction if $l_1$ is large. However, when the excitation energy $\epsilon$ above the Fermi level decreases then $\rho_2$ becomes smaller and it approaches the one-particle density $\rho$ at low energy: $\rho_2 \approx \epsilon^2 \rho$. As a result the value of $\kappa$ also drops with $\epsilon$ so that the delocalization of TIP pairs practically disappears near the Fermi energy. This has been shown in [4,5] in the approximation of the frozen Fermi sea created by fermions. Recent numerical studies of TIP pairs with short range interaction near the Fermi level [14] confirmed these theoretical expectations.

FIG. 1. Probability distributions $f$ and $f_d$ for TIP in 2d disordered lattice of size $L = 40$, and interaction of radius $R = 12$ and width $\Delta R = 1$. Left column, one-particle probability $f$ for $W = 8V$: ground state at $U = 0$ (top); ground state with binding energy $\Delta E = -1.05V$ at $U = -2V$ (middle); coupled state with $\Delta E = -0.19V$ at $U = -2V$ (bottom). Right column: $f$ for coupled state, compare to bottom left, at $W = 12V$ and $U = -2V$ with $\Delta E \approx -0.19V$ (top); inter-particle distance probability $f_d$ related to the middle left case (middle); $f_d$ related to the bottom left case (bottom). All data are shown for the same disorder realisation. Color 2d density plots for these data are given in Fig. 1bis of Appendix.
In this paper we discuss another type of situation in which TIP delocalization (see Fig. 1) takes place mainly due to geometrical reasons and not due to the relation $\rho_2 \gg \rho$. As a result the TIP pair can be delocalized in a close vicinity to the Fermi level that opens new interesting possibilities for interaction induced delocalization in the localized noninteracting phase. To study this new situation we investigate a model with a long range attractive interaction between particles in the 2d Anderson model. In this case the particles can rotate around their center of mass, being far from each other and keeping the same energy, while the center can move randomly in two dimensions. As a result the system has effectively three degrees of freedom that makes it rather similar to the case of one particle in the 3d Anderson model where delocalization takes place at sufficiently weak disorder. A somewhat similar situation has been studied recently for particles with Coulomb interaction but only excited states were considered there and the delocalization was attributed to the large ratio $\rho_2/\rho$ [7]. Here we show that in fact the conditions for delocalization are much less restrictive.

To illustrate the above ideas let us first discuss the case of only two particles with attractive interaction $U(r) < 0$ in the 2d Anderson model described by the Schrödinger equation

$$E_{n_1} + E_{n_2} + U(n_1 - n_2)\psi_{n_1,n_2} + V(\psi_{n_1+1,n_2} + \psi_{n_1-1,n_2} + \psi_{n_1,n_2+1} + \psi_{n_1,n_2-1}) = E\psi_{n_1,n_2}. \tag{1}$$

Here $n_{1,2}$ are the indices of the two particles on the 2d lattice with $L^2$ sites and periodic boundary conditions, $V$ is the hopping between nearby sites and the random on-site one-particle energies $E_{n_{1,2}}$ are homogeneously distributed in the interval $[-W/2, W/2]$. The long range attractive interaction depends only on the distance between particles $r = |n_1 - n_2|$ and is equal to a constant $U < 0$ if $|r - R| \leq \Delta R$ and zero otherwise. The value of $r$ is determined as the minimal inter-particle distance on the periodic lattice. Thus the interaction takes place only inside a ring of radius $R$ and width $\Delta R$, and we assume that $R \gg \Delta R \geq 1$. For $U = 0$ the eigenstates are given by the product of two one-particle (noninteracting) eigenstates which are always localized in 2d in a presence of disorder [6].

In the limit of very strong attractive interaction $|U| \gg V$ the TIP coupled states form the energy band of width $\Delta \approx 16V$ around $E \simeq -|U|$ (we consider only the states symmetric in respect to particle interchange). For states in this band the particles are located always inside the ring which center can move over the 2d lattice. Since $|U| \gg V$ these states are decoupled from all other states with particles outside the ring. In the ring the Schrödinger equation is in fact rather similar to the case of 3d Anderson model of one particle. In this analogy the number of sites inside the ring $M_R \approx 2\pi R \Delta R$ determines the effective number of 2d planes placed one over another in the third $z$-dimension (length size $L_z = M_R$).

In this 3d model the effective strength of disorder is approximately $2W$ since the diagonal term is now the sum of two $E_n$ values. Also one site is coupled with $Z = 8$ neighbours contrary to $Z = 6$ for 3d case (assuming $\Delta R \gg 1$). Since in 3d the Anderson transition at the band center takes place at $W_c = 2.75ZV = 16.5V$ [7], we expect that TIP states inside the ring will be delocalized in the middle of the band when $2W/ZV = 2.75$ that gives the transition at $W_{c2} \approx 11V$. This estimate is in agreement with numerical simulations of the model [8]. Of course, since the size in the third direction is finite the eigenstates will be eventually localized. But their localization length $l_c$ will make a sharp jump from $l_c \sim 1$ at $W > W_{c2}$ to $l_c \sim \exp(g) \gg 1$ at $W < W_{c2}$ that follows from the standard scaling theory in 2d [9,12,13]. Here $g$ is the conductance of the quasi-two-dimensional layer of width $L_z = M_R$. As usual $g = E_c/\Delta_1$ where $E_c = D/L^2$ is the Thouless energy, $\Delta_1 \sim V/(L^2 L_z)$ is the level spacing [8] and the diffusion rate in the lattice model is $D \sim V(W/V)^2$. As a result for $W < W_{c2}$ the TIP delocalization length jumps to exponentially large value $l_c \sim \exp(2\pi R \Delta R/W_{c2}^2 V)$. In these estimates we assumed that $l_1 > \Delta R > l_1$ since if $\Delta R \gg l_1$ the majority of states inside the ring are noninteracting and can be presented as the product of one-particle eigenstates. We also note that for $W < W_{c2}$ there is an energy interval around the band center with delocalized states where the TIP ring diffuses with the rate $D \sim V(W_{c2}/V)^2$. When $W$ decreases the mobility edge approaches the bottom of the band as it happens in 3d Anderson model.

The above arguments presented for the case $|U| \gg V$ indicate that it is possible to have a similar TIP delocalization at moderate value of $U \sim V$ near the Fermi level. To investigate this case we rewrite the equation (1) in the basis of the noninteracting eigenstates 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 $\chi_{m_1,m_2}$ are eigenfunctions of the TIP problem written in the basis of one-particle eigenstates $\phi_n$ with eigenenergies $E_n$. The matrix $UQ_{m_1,m_2,m_1',m_2'}$ represents the two-body matrix elements of interaction $U(n_1 - n_2)$ between noninteracting eigenstates $|\phi_{m_1}\phi_{m_2}\rangle$ and $|\phi_{m_1'}\phi_{m_2'}\rangle$. The Fermi sea is determined by the restriction of the summation in (2) to $m_1'' > 0$ with energies $E_{m_1''} > E_F$, where $E_F$ is the Fermi energy related to the filling factor $\mu$. We choose the case with half filling $\mu = 1/2$ for which $E_F \approx 0$. In this way our model corresponds to the approximation of frozen Fermi sea successfully used for the Cooper problem [10]. As it was done by Cooper we also introduce the high energy cut-off defined by the condition $1 \leq m_1' + m_2' \leq M$. This rule
determines an effective phonon frequency $\omega_D \propto M/L^2$. We fix $\alpha = L^2/M \approx 15$ since $\omega_D$ should be independent of the system size $L$ [24]. We checked that the results are not affected by a variation of $\alpha$ in few times. The first studies of the TIP model with frozen Fermi sea was done by Imry [5] with the aim to take into account the effect of finite fermionic density and then was also analyzed in [3]. Recently a similar model was investigated for the case of Hubbard attraction in 3d [14].

For $U = -2V$, $W = 8V$ and $\Delta R = 1$: $L = 20$ ($\circ$), $L = 22$ (triangle down), $L = 26$ (diamond), $L = 30$ (triangle up), $L = 40$ (square); full/empty symbols are for $R = 8/R = 12$; the shaded band shows the variation of $\xi$ at $E_F$ and $U = 0$ for $20 \leq L \leq 40$. Insert shows dependence of $\xi$ on disorder $W/V$ at $R = 8$ for the ground state at $U = -2V$, $L = 30$ ($\times$) and at $U = 0$, $L = 30$ (+), and for the states at the delocalization border with binding energy $\Delta E \approx \Delta E_c$ at $U = -2V$ ($\ast$).

To study the eigenstate properties of our model we diagonalize numerically the Hamiltonian (3) and rewrite the eigenfunctions in the original lattice basis. In this way we determine the two-particle probability distribution $F(n_1, n_2)$ from which we extract the one particle probability $f(n_1) = \sum_n F(n_1, n_2)$ and the probability of inter-particle distance $f_d(r) = \sum_{n_2} F(r + n_2, n_2)$ with $r = n_1 - n_2$. The binding energy of an eigenstate in (3) is $\Delta E = E - 2E_F \approx E$ since $E_F \approx 0$. For the ground state with energy $E_g$ the coupling energy is $\Delta = 2E_F - E_g$. The typical examples of probability distributions are shown in Fig. 1. They clearly show that the ground state in the presence of interaction remains localized and the particles stay on distance $R$ from each other. However, there are states with negative binding energy ($\Delta E < 0$) which are delocalized by interaction and for which the particles move around the ring in agreement with discussion of model [11] at $|U| \gg V$. We stress that this delocalization of coupled states ($\Delta E < 0$) takes place in the well localized one-particle phase. However, at very strong disorder this delocalization disappears (see top right case in Fig. 1).

To analyze the delocalization of states with negative binding energy $\Delta E$ in a more quantitative way we determine the inverse participating ratio (IPR) $\xi$ for one-particle probability $1/\xi = \langle \sum_n f^2(n) \rangle$, where brackets mark the averaging over 100 disorder realisations. In this way $\xi$ gives the number of lattice sites occupied by one particle in an eigenstate. The dependence of $\xi$ on $\Delta E$ and $W$ is shown in Fig. 2 for different lattice sizes $L$ in the presence of interaction. This figure shows that near the ground state the interaction creates states which are even more localized than in the absence of interaction ($\xi$ is significantly smaller than at $U = 0$, see insert Fig. 2).

In fact for $-\Delta < \Delta E < \Delta E_c < 0$ the IPR value even slightly drops with the increase of $L$. However for the states with binding energy $\Delta E_c < \Delta E < 0$ the situation becomes different and $\xi$ grows significantly with $L$ while the change of IPR at $U = 0$ with $L$ is rather weak (see shaded band in Fig. 2). The critical value of the binding energy $\Delta E_c$ can be defined as such an energy at which $\xi$ remains independent of $L$. In this way $\Delta E_c$ determines the mobility edge for coupled states so that at given $U$ and $W$ the TIP eigenstates are localized for $-\Delta < \Delta E < \Delta E_c$ while for $\Delta E_c < \Delta E < 0$.
the states becomes delocalized (see an example in Fig. 1). In agreement with this picture $\xi$ varies up to 30 times when $\Delta E$ changes from $-\Delta$ up to 0. This variation grows with $L$ and the interaction radius $R$ since the system becomes more close to the effective 3d Anderson model as it was discussed above. The qualitative change of the structure of the eigenstates leads also to a change in the level spacing statistics $P(s)$ (Fig. 3). Near the ground state the statistics is close to the Poisson distribution $P(s) = \exp(-s)$ typical for the localized Anderson phase \[^{21}\] while for $\Delta E < \Delta E < 0$ it approaches to the Wigner surmise $P_W(s) = \pi s \exp(-\pi s^2/4)/2$ corresponding to the delocalized phase \[^{22}\].

![Image](http://w3-phystheo.ups-tlse.fr/~dimar)

FIG. 4. Dependence of the delocalization border $\Delta E_c$ and the binding energy of the ground state $-\Delta$ on disorder $W/V$. The values of $\Delta E_c$ are shown by (●) for $U = -V$ / $-2V$; the values of $-\Delta$ are shown by upper/lower dashed line for $U = -V$ / $-2V$ and $L = 30$ (vertical intervals give variation for $20 \leq L \leq 30$).

The variation of the delocalization border $\Delta E_c$ for TIP coupled states with disorder strength and interaction is shown in Fig. 4. While the coupling energy $\Delta$ grows with $U$ and $W$, the mobility edge $\Delta E_c < 0$, on the contrary, disappears at strong $W$. According to the data of Fig. 4 all states with binding energy $\Delta E < 0$ become localized for $W > W_{c2} \approx 9.5V$ ($U = -2V$) and $W > W_{c2} \approx 8V$ ($U = -V$). This shows that at weaker interaction a weaker disorder is required to have delocalized coupled states. As it follows from Fig. 4, at small disorder $W$ the delocalization border $\Delta E_c$ becomes closer and closer to the ground state. This means that at weak disorder the delocalization will take place for excited states with low energy. For $W \ll W_{c2}$ and $U \sim -V$ the diffusion rate of delocalized TIP ring can be estimated as $D_2 \sim V(W_{c2}/W)^2$ \[^{22}\]. Further studies are required to determine the dependence of $W_{c2}$ on $W$ at $|U| \ll V$.

In conclusion, our results show that long range attractive interaction between two particles in 2d leads to the appearance of delocalized diffusive states near the Fermi level inside the well localized noninteracting phase. It would be interesting to understand what will be the consequences of this delocalization for real many-body fermionic problem with attractive interaction. It is possible that obtained results will be also relevant for electrons with Coulomb repulsion. Indeed, in this case at very weak disorder each electron oscillates near an equilibrium position and the two-body interaction can be considered as an effective harmonic attraction \[^{23}\].

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FIG. 1bis. Color 2d density plots for the data of Fig.1 with the same ordering of figures. Blue corresponds to the minimum of the probability distribution and red to the maximum. The first four figures are drawn in logarithmic scale while two figures at the bottom are in linear scale. Blue/Red color corresponds to: $f = 1.3 \times 10^{-10}/f = 0.2$ (top left), $f = 1.1 \times 10^{-9}/f = 0.26$ (middle left), $f = 1.5 \times 10^{-9}/f = 0.014$ (bottom left), $f = 1.14 \times 10^{-11}/f = 0.073$ (top right), $f_d = 3.8 \times 10^{-7}/f_d = 0.1$ (middle right), $f_d = 1.5 \times 10^{-5}/f_d = 0.0032$ (bottom right).