Two interacting quasiparticles above the Fermi sea

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We study numerically the interaction and disorder effects for two quasiparticles in two and three dimensions. The dependence of the interaction-induced Breit-Wigner width $\Gamma$ on the excitation energy $\epsilon$ above the Fermi level, the disorder strength and the system size is determined. A regime is found where $\Gamma$ is practically independent of $\epsilon$. The results allow to estimate the two quasiparticle mobility edge.

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Recently the combined effect of interaction and disorder has been studied by different groups for two particles in a random potential \[1\] \[2\]. These researches showed an interaction-induced enhancement of the two-particle localization length $l_c$ compared to the non-interacting length $l_1$. For low-dimensional systems (1d, 2d) the two interacting particles (TIP) can propagate coherently over a large distance $l_c \gg l_1$, but still remain localized. In 3d, the interaction can lead to TIP delocalization in an otherwise completely localized regime. In physical systems however one should study the interaction effect at finite particle density. This type of problem is much more difficult for both the analytical and numerical approaches. Up to now the only theoretical treatment of this case has been done by Imry \[2\]. He took into account the effect of the Fermi sea on the interaction-induced delocalization of two quasiparticles. According to Imry’s estimate in 3d the two quasiparticle mobility edge is lower compared to the non-interacting one. So far only the 1d case has been treated numerically \[2\]. However, this case is of lesser importance since the enhancement is recovered quite far above the Fermi level contrarily to the 2d and 3d cases. Therefore it is very important to study the problem in higher dimensions.

Exact numerical computations at finite density are quite heavy and due to that only small system sizes are accessible \[3\]. Even though this approach has led to a number of interesting results, it seems that size restrictions would not allow to check the Imry estimate since it requires a relatively large one-particle localization length $l_1$. Therefore we chose another approach which is based on the computation of the interaction-induced Breit-Wigner width $\Gamma$ of the local density of states of two interacting quasiparticles (TIQ) above the Fermi sea. This width plays an important role since it is directly related to the enhancement factor for the localization length $\eta \sim \Gamma \rho_c$, where $\rho_c$ is the density of states coupled by the interaction \[2\] \[4\]. Also $\Gamma$ strongly affects the $\Sigma_2(E)$-statistics on energy scale $E > \Gamma$ \[10\]. Such $\Gamma$-based approach even though not direct is much more efficient and allowed to get a better understanding of TIP localization in the 1d case \[1\]. To facilitate the numerical simulations we used the approximation proposed in \[3\] \[4\] \[11\] based on the consideration of only two quasiparticles above the Fermi energy $E_F$ neglecting all TIQ transitions involving hole excitations below $E_F$. With such an approximation the quasiparticle lifetime becomes infinite or in other words the inelastic processes are suppressed (see discussion below). In this context we are able to study the TIQ problem in blocks of linear size up to $L = 30$ in 2d and $L = 10$ in 3d which are significantly larger than in exact diagonalization of multiparticle problems. Our approach can also give a better understanding of the problem of quasiparticle interactions in a quantum dot which has been recently addressed experimentally \[12\] and theoretically \[13\].

For numerical studies we chose the TIQ model with on-site interaction of strength $U$ on the 2d/3d Anderson lattice with intersite hopping $V$ and diagonal disorder homogeneously distributed in the interval $[-W, W]$. The eigenvalue equation expression in the basis of two-particle unperturbed eigenstates reads

\[ (E_{m_1} + E_{m_2}) \chi_{m_1,m_2} + U \sum_{m_1',m_2'} Q_{m_1,m_2,m_1',m_2'} \chi_{m_1',m_2'} = E \chi_{m_1,m_2} \quad (1) \]

where $R$ determines the transformation between the lattice sites basis $|n\rangle$ and the one-particle eigenbasis $\phi_m$ with eigenenergies $E_m$ so that $|n\rangle = \sum_m R_{n,m} \phi_m$. Accordingly $\chi_{m_1,m_2}$ are eigenfunctions of the TIQ problem in one-particle eigenbasis. The matrix of transitions produced by the interaction is $Q_{m_1,m_2,m_1',m_2'} = \sum_n R_{n,m_1} R_{n,m_2} R_{n,m_1'} R_{n,m_2'}$. The Fermi sea is introduced by restricting the sum in (1) to $m_1' < m_2$ with unperturbed energies $E_{m_1'} > E_F$. The value of $E_F$ is determined by the filling factor $\mu$ which was fixed at $\mu = 1/4$ in 2d and $\mu = 1/3$ in 3d. However the results are not sensitive to this choice. At small disorder this gives approximately $E_F \approx -1.4V$ and $E_F \approx -V$ respectively. Due to the on-site nature of the interaction, only symmetric configurations were considered. By direct diagonalization of...
the model (1) we computed the local density of states

$$\rho_{W}(E - E_{m_1} - E_{m_2}) = \sum_{\lambda} |\chi_{m_1, m_2}^{(\lambda)}|^2 \delta(E - E_{\lambda}) \quad (2)$$

This function characterizes the probability contribution of eigenfunction $\chi_{m_1, m_2}^{(\lambda)}$ with eigenenergy $E_{\lambda}$ in the unperturbed basis $\{|\phi_{m_1}, \phi_{m_2}|\}$. Generally we found that it has the well-known Breit-Wigner shape $\rho_{BW}(E) = \Gamma / (2\pi(E^2 + \Gamma^2 / 4))$ (see Fig.1) where the width $\Gamma$ depends on the parameters of the model. Our main aim was to investigate this dependence on the system size, the interaction strength and the TIQ excitation energy $\epsilon = E - 2E_F$ above the Fermi sea.

FIG. 1. Energy dependence of the rescaled Breit-Wigner width $\Gamma / \Gamma_0$ in 2d. Direct diagonalization (DD) data at $W/V = 1$ with $L = 15$ (triangles), $L = 20$ (squares); $U/V = 1.5$ and $L = 20$ (diamonds). Fermi golden rule (FGR) data: $W/V = 1$ with $L = 20$ (+), $L = 25$ (x); $W/V = 0.5$ with $L = 15$ (*). The straight line $\Gamma(\epsilon) / \Gamma_0 = C\epsilon / V$ with $C = 0.52$ shows the Imry estimate. Upper inset: the same in a log-log scale with FGR data at higher disorder $W/V = 3$ (left) and $W/V = 5$ (right) triangles ($L = 30$). Lower inset: $\rho_{W}$ vs. $E$ for $L = 20, W = V = 1, U = 0.6, \epsilon = 0.4$ fitted by $\rho_{BW}$ with $\Gamma = 0.18\Gamma_0$ (solid curve).

The results for the 2d, 3d cases in the regime of weak disorder are presented in Figs.1, 2. For sufficiently high excitation energy $\epsilon$, the restriction imposed by the Fermi sea becomes unimportant and the width $\Gamma(\epsilon)$ tends to the value $\Gamma_0 = U^2 / (V L^d)$ which corresponds to the result obtained with ergodic eigenfunctions [1][3][4]. In this approach the transition matrix elements have a typical value $U^2 = U^2 Q^2 \sim U^2 / L^{3d}$ and the transition rate is given by the Fermi golden rule with $\Gamma_0 \sim U^2 Q^2 \rho_c \sim L^{2d} / V$. The presence of the Fermi sea modifies this density which becomes energy-dependent $\rho_c(\epsilon) \sim L^{2d} \epsilon / V^2$. As a result the width $\Gamma$ drops with decreasing energy as

$$\Gamma(\epsilon) = C T_0 \frac{\epsilon}{V} = C \frac{U^2 \epsilon}{V^2 L^d} \quad (3)$$

This behaviour was assumed to remain valid for weak enough disorder as long as $L \leq l_1$. Hence $\Gamma$ is independent on the disorder strength $W$. Indeed for $l_1 > L$ this estimate is in good agreement with the numerical data presented in Figs.1, 2 with $C = 0.52$ (2d) and $C = 0.3$ (3d). Most of the data for $\Gamma$ in Figs.1, 2 were obtained by direct diagonalization of the model (1). Another way to determine $\Gamma$ without computation of the TIQ eigenstates is based on the Fermi golden rule which should remain valid for moderate interaction strength. This approach gives $\Gamma = 2 \pi \sum_{m_1, m_2} |UQ_{m_1, m_2}|^2 \delta(\epsilon + 2E_F - E_{m_1} - E_{m_2})$ in terms of the transition matrix elements between one-particle eigenstates only. Here $\epsilon = E_{m_1} + E_{m_2} - 2E_F$ and to improve the statistics we averaged over different $n_{1,2}$ with approximately the same $\epsilon$. As can be seen in Figs.1, 2, both methods are in good agreement for interaction strength $U \leq 1.5V$. Another confirmation of the validity of the golden rule is the $U^2$-dependence of $\Gamma$ obtained by direct diagonalization (Fig.2). Both approaches confirm also the scaling $\Gamma \propto L^{-d}$ valid for weak disorder. We used up to 100 realizations of disorder for the Fermi golden rule approach and up to 500 for direct diagonalization.

FIG. 2. Same as Fig.1 in 3d. DD data at $U/V = 1.2$ and $W/V = 2$ with $L = 4$ (o), $L = 5$ (squares), $L = 6$ (diamonds) and $L = 7$ (triangles). FGR data: $W/V = 2$ with $L = 10$ (x); $W/V = 1$ with $L = 8$ (+). Here $C = 0.3$. Upper inset: the same in a log-log scale with FGR data at higher disorder $W/V = 6$ (left) and $W/V = 10$ (right) triangles ($L = 30$). Lower inset: FGR data for $\Gamma$ vs. $U/V$ at $W/V = 2, L = 6, V = \epsilon = 0.5$ (solid line: $\Gamma = 0.3 \Gamma_0$).

The situation becomes more intricate at higher disorder. Here our results show that $\Gamma$ becomes much less sensitive to $\epsilon$ variation (Figs.3). There is a clear tendency that at still moderate disorder $\Gamma$ becomes practically independent on $\epsilon$ which has been varied over one order of magnitude. In the 3d case, such behaviour takes place even in the delocalized regime $W < W_c \approx 8.2V$. The data even indicate a small growth of $\Gamma(\epsilon)$ with decreasing $\epsilon$ at $W \geq 6V$. At high disorder $l_1$ decreases and becomes comparable or even less than $L$. In this situation the eigenstates are no longer ergodic in the block and the scaling $\Gamma \propto L^{-d}$ is no more valid. In the limit $1 < l_1 \ll L$,
it is natural to expect another scaling $\Gamma \propto l_{\text{crit}}^{-d}$. To check this scaling we computed the inverse participation ratio (IPR) $\xi \sim l_{\text{crit}}^d$ which allowed to calculate the ergodic value $\Gamma_1 = U^2/(V\xi)$.

![Graph showing energy dependence of the rescaled Breit-Wigner width $\Gamma/\Gamma_1$ in 2d (left) and 3d (right).]

**FIG. 3.** Energy dependence of the rescaled Breit-Wigner width $\Gamma/\Gamma_1$ in 2d (left) and 3d (right). FGR data in 2d: $W/V = 1$ with $L = 20$ (o) and $L = 30$ (points); $W/V = 2$ with $L = 20$ (open squares) and $L = 30$ (full squares); $W/V = 3$ with $L = 20$ (open diamonds) and $L = 30$ (full diamonds). DD data in 2d at $L = 20$, $U/V = 0.6$: $W/V = 1$ (+), $W/V = 2$ (x) and $W/V = 3$ (*). FGR data in 3d at $L = 10$: $W/V = 2$ (o), $W/V = 6$ (squares), $W/V = 10$ (diamonds) and $W/V = 14$ (triangles). DD data in 3d at $L = 6$, $U/V = 1.2$: $W/V = 2$ (+) and $W/V = 6$ (x).

At sufficiently high excitation energy, the real width should be $\Gamma \sim \Gamma_1$ which gives the correct scaling with system size in the localized regime according to the numerical data. This would explain why in the block of fixed size $\Gamma$ increases with increasing disorder (see inserts in Figs.1, 2). While such estimate gives the correct value of the width $\Gamma_1 = U^2/(V\xi)$, it does not explain the change of energy dependence with disorder. We should note that even in this unusual regime the two-particle density of states $\rho_2$ definitely show that it increases linearly with the excitation energy $\epsilon$ as $\rho_2 \sim \epsilon/\Delta^2$. Therefore the only possibility is that at higher disorder the ergodic estimate for $U_s$ is no longer valid. Indeed from the theory of quasiparticle lifetime in disordered metals and quantum dots [13,14,15] it is known that the diffusive nature of the dynamics should be taken into account. For excitation energy $\epsilon > E_c$ much bigger than the Thouless energy $E_c$, the quasiparticle decay rate is $\Gamma_D \sim U_s^2 \rho_2 \sim \Delta(U\epsilon/V^2E_c)^{d/2}$ where $\rho_2 \sim \rho_3 \epsilon/\Delta$ is the density of three-particle states composed of two particles and one hole in the final state. In the other regime relevant for the metallic quantum dot $\Delta < \epsilon < E_c$ this rate is $\Gamma_D \sim \Delta(U\epsilon/V^2E_c)^{d/2}$ [13]. This shows that the matrix elements $U_s^2 \sim \Gamma_D/\rho_3$ are not always given by the ergodic estimate in agreement with recent results [13]. The different numerical regimes may be described by the following approximate expression [13]:

$$U_s^2 \sim \left(\frac{U}{V}\right)^2 \frac{\Delta^2}{g^2} \left(1 + \frac{\epsilon}{E_c}\right)^{d/2-2}$$

(4)

where $g = E_c/\Delta$ is the conductance assumed to be much bigger than one. According to (4) the TIQ width $\Gamma \sim U_s^2/\rho_3$ increases with disorder $W$ even in the metallic regime since $E_c = D/L^2 \sim V^3/(WL)^2$ with $D$ being the diffusion constant. The ergodic estimate for $U_s^2$ is recovered for $g > E_F/\Delta \sim V/\Delta$ [16] corresponding to very weak disorder. While the exact numerical coefficients in (4) are not known, it gives the energy-dependence $\Gamma \propto \epsilon^{d/2-1}$ which is in agreement with the numerical data for $d = 2$ (Fig.3) but in 3d the data indicate an algebraic dependence with power $\alpha < 0$ ($\alpha \approx -0.2$ for $W = 6V$ and $\alpha \approx -0.3$ for $W = 10V$) instead of the theoretical value $\alpha = 1/2$. There can be different reasons for this discrepancy. One case $W = 10V$ corresponds to the localized regime while the theory requires a metallic behaviour. The other case $W = 6V$, even though still delocalized, is quite close to the critical value $W_c$. Our data indicate that in the metallic regime with $1 < W/V < 6$ the power $\alpha$ smoothly changes from 1 to -0.3.

Surprisingly at present there are no theoretical predictions for $U_s^2$ not only near the critical value $W_c$ but also in the localized regime with $l_1 \ll 1$. It seems natural to make the assumption that in the localized case, the transition matrix elements will be given by an equation similar to (4) with $g \approx 1$ since in a block of size $l_1$ the Thouless energy is $E_c \approx \Delta \sim V/l_1^2$. This gives $\Gamma \approx \Gamma_1(\epsilon/\Delta)^{\alpha}$ where $\alpha$ has replaced the theoretical value $d/2-1$ valid in the metallic regime. We will assume that for $d \geq 2$ the exponent $\alpha < 1$. In 3d the TIQ mobility edge $\epsilon_{m2}$ is defined by the condition $\kappa = \Gamma \rho_2 > 1$ [13]. Since $\rho_2 \sim \epsilon/\Delta^2$ the above expressions for $\Gamma$ give

$$\epsilon_{m2} \sim \frac{V_{\text{crit}}}{U} \left(\frac{V}{U}\right)^{2/(1+\alpha)} \sim V \left(\frac{\epsilon_{m1}}{V}\right)^{\nu d} \left(\frac{V}{U}\right)^{2/(1+\alpha)}$$

(5)

where $\epsilon_{m1} \sim V_{\text{crit}}^{-1/\nu}$ is the one-particle mobility edge. The one-particle critical exponent is $\nu \approx 1.5$. Due to that for $U \sim V$, the edge $\epsilon_{m2} \ll \epsilon_{m1}$. The above result (5) gives for $\epsilon_{m2}$ a much smaller value than the one given by the Imry estimate [13]. The main reason for this is that the transition matrix elements in the block of size $l_1$ where $g \approx 1$ are much larger than their ergodic value used in [13]. The condition that the TIQ delocalization border in $U$ at $\epsilon \sim V$ is the same as for TIP ($U > V/l_1^{d/2}$ [13]) gives $\alpha = 0$.

The numerical results for the dependence of $\kappa = \Gamma \rho_2\epsilon$ on $\epsilon$ are presented in Fig.5. To determine numerically the
density of coupled states $\rho_c \sim \epsilon^2 d/V^2$ in the localized regime we computed it taking into account only those TIQ states which give contributions larger than 30% of the value of $\Gamma$ (the data were not sensitive to the cut-off value). The density $\rho_c$ defined in this way is independent of the system size when $L > l_1$. The data show that for $W = 14V$ there is no TIQ delocalization ($\kappa < 1$). However closer to the one-particle delocalization border but still above it ($W > W_c$) the value of $\kappa$ becomes bigger than one at moderate excitation energies and TIQ delocalization should take place. Further investigations are required to check more accurately the theoretical prediction (5) for the mobility edge $\epsilon_{m2}$.

In conclusion we analyzed the interaction-induced delocalization of two quasiparticles above the Fermi sea in the approximation where inelastic processes are suppressed. According to our numerical results and semi-analytical estimates, the TIQ mobility edge is below the one-particle edge ($\epsilon_{m2} < \epsilon_{m1}$). The obtained value of $\epsilon_{m2}$ is even much smaller than the value proposed in [4] due to the fact that transition matrix elements are much bigger than their ergodic value near the Fermi level.

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