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 Γ on the excitation energy above the Fermi level (ϵ), the disorder strength, and the system size are determined. A regime is found where Γ is practically independent of ϵ. The results allow us to estimate the two quasiparticle mobility edge. [S0031-9007(97)03500-X]

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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 [1–5]. This research showed an interaction-induced enhancement of the two-particle localization length l_c compared to the noninteracting 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 a 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 mobility edge for two interacting quasiparticles is lower than that for noninteracting quasiparticles. So far only the 1D case has been treated numerically [6]. However, this case is of less importance since the enhancement occurs very far above the Fermi level, in contrast to the 2D and 3D cases. Therefore it is very important to study the problem in higher dimensions.

Exact numerical computations at a finite density are quite difficult, and for this reason only small system sizes are accessible [7,8]. Even though this approach has led to a number of interesting results, it seems that size restrictions do not allow a check of the Imry estimate since it requires a relatively large one-particle localization length l_1. Therefore we choose another approach that is based on a computation of the interaction-induced Breit-Wigner width Γ 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 $\kappa \sim \Gamma\rho_c$, where ρ_c is the density of states coupled by the interaction [1,2,9]. Γ also strongly affects the $\Sigma_2(E)$ statistics on the energy scale $E > \Gamma$ [10]. Such a Γ-based approach, even though not direct, is much more efficient and allows us to get a better understanding of TIP localization in the 1D case [11]. To facilitate the numerical simulations we used the approximation proposed in [2,4,6] that is 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 decay rate Γ_D becomes zero or, in other words, the inelastic processes are suppressed (see the discussion below). In this context we are able to study the TIQ problem in blocks of linear sizes up to $L = 30$ in 2D and $L = 10$ in 3D, which are significantly larger than for the 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 the numerical studies, we chose the TIQ model with an on-site interaction of strength U on the 2D/3D Anderson lattice with intersite hopping V and the diagonal disorder homogeneously distributed in the interval $[-W/2, W/2]$. The eigenvalue equation expressed in the basis of the two-particle unperturbed eigenstates reads

$$(E_{m_1} + E_{m_2})\chi_{m_1,m_2} + U \sum_{m_1',m_2'} Q_{m_1,m_2,m_1',m_2'}\chi_{m_1',m_2'} = E\chi_{m_1,m_2}\,. \tag{1}$$

Here, the transformation R between the lattice sites basis $|n\rangle$ and the one-particle eigenbasis ϕ_m with eigenenergies E_m is given by $|n\rangle = \sum_m R_{n,m}\phi_m$. Accordingly, χ_{m_1,m_2} are eigenfunctions of the TIQ problem in the 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 $m'_{1,2}$ with unperturbed energies $E_{m'_{1,2}} > E_F$. The value of E_F is determined by the filling factor μ 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 a small disorder this gives approximately $E_F \approx -1.4V$ and $E_F \approx -V$, respectively. Because of the on-site nature of the interaction, only symmetric configurations were considered. By direct diagonalization of the model (1) we computed the

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local density of states,

$$\rho_W(E - E_{m_1} - E_{m_2}) = \sum_\lambda |\chi^{(\lambda)}_{m_1,m_2}|^2 \delta(E - E_\lambda). \quad (2)$$

This function characterizes the probability contribution of the eigenfunction $\chi^{(\lambda)}_{m_1,m_2}$ with eigenenergy E_λ in the unperturbed basis $|\phi_{m_1}\phi_{m_2}\rangle$. We found that it generally has the well-known Breit-Wigner shape $\rho_{BW}(E) = \Gamma/[2\pi(E^2 + \Gamma^2/4)]$ (see Fig. 1), where the width Γ 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 above the Fermi sea, $\epsilon = E - 2E_F$.

The results for the 2D and 3D cases in the regime of weak disorder are presented in Figs. 1 and 2. For a sufficiently high excitation energy ϵ, the restriction imposed by the Fermi sea becomes unimportant and the width $\Gamma(\epsilon)$ tends to the value $\Gamma_0 = U^2/VL^d$ which corresponds to the result obtained with the ergodic eigenfunctions [1,2,9]. In this approach the transition matrix elements have a typical value $U_s^2 = U^2Q^2 \sim U^2/L^{3D}$, and the transition rate is given by the Fermi golden rule with $\Gamma_0 \sim U^2Q^2\rho_c$ and $\rho_c \sim L^{2D}/V$. 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 Γ drops with decreasing energy as [2]

$$\Gamma(\epsilon) = C\Gamma_0 \frac{\epsilon}{V} = C \frac{U^2\epsilon}{V^2L^d}. \quad (3)$$

This behavior was assumed to remain valid for a weak enough disorder as long as $L \le l_1$. Hence Γ is independent of the disorder strength W. Indeed, for $l_1 \gg L$ this estimate is in good agreement with the numerical data presented in Figs. 1 and 2 with $C = 0.52$ (2D) and $C = 0.3$ (3D). Most of the data for Γ in Figs. 1 and 2 were obtained by direct diagonalization of the model (1). Another way to determine Γ without computation of the TIQ eigenstates is based on the Fermi golden rule which should remain valid for a moderate interaction strength. This approach gives $\Gamma = 2\pi \sum_{m_1',m_2'} |UQ_{m_1,m_2;m_1',m_2'}|^2 \delta(\epsilon + 2E_F - E_{m_1'} - E_{m_2'})$ 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 $m_{1,2}$ with approximately the same ϵ. As can be seen in Figs. 1 and 2, both methods are in good agreement for the interaction strength $U \le 1.5V$. Another confirmation of the validity of the golden rule is the U^2 dependence of Γ obtained by direct diagonalization (Fig. 2). Both approaches also confirm that the scaling $\Gamma \propto L^{-d}$ is valid for weak disorder. We used up to 100 realizations of disorder for the Fermi golden rule approach and up to 500 for the direct diagonalization.

The situation becomes more intricate at higher disorder. Here our results show that Γ becomes much less sensitive to the ϵ variation (Fig. 3). The tendency is clear: At a disorder which is still moderate, Γ becomes practically independent of ϵ, which has been varied over 1 order of magnitude. In the 3D case, such behavior takes place even in the delocalized regime $W < W_c \approx 16.3V$. The data even indicate a small growth of $\Gamma(\epsilon)$ with decreasing ϵ at $W \ge 12V$. At high disorder l_1 decreases and becomes comparable with or even less than L. In this situation the eigenstates are no longer ergodic in the

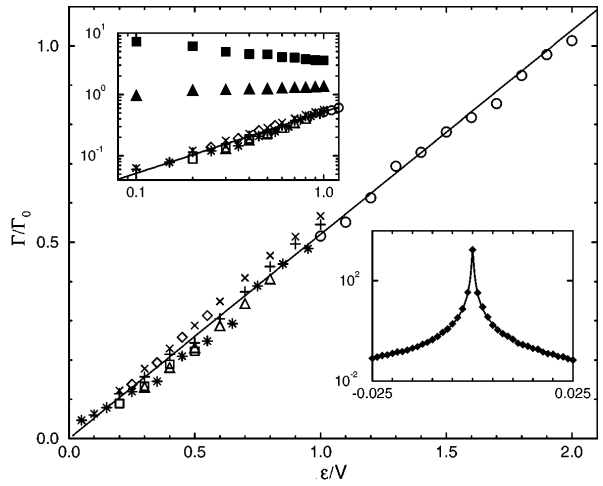

FIG. 1. Energy dependence of the rescaled Breit-Wigner width Γ/Γ_0 in 2D. Direct diagonalization (DD) data at $W/V = 2$: $U/V = 0.6$ with $L = 8$(○), $L = 15$ (△), $L = 20$ (□); $U/V = 1.5$ and $L = 20$ (◇). Fermi golden rule (FGR) data: $W/V = 2$ with $L = 20$ (+), $L = 25$ (×); $W/V = 1$ with $L = 15$ (∗). The straight line $\Gamma(\epsilon)/\Gamma_0 = C\epsilon/V$ with $C = 0.52$ shows the Imry estimate. Upper inset: the same on a log-log scale with FGR data at higher disorders [$W/V = 6$ (▲) and $W/V = 10$ (■) ($L = 30$)]. Lower inset: ρ_W vs E for $L = 20, W/2 = V = 1, U = 0.6, \epsilon = 0.4$ fitted by ρ_{BW} with $\Gamma = 0.18\Gamma_0$ (solid curve).

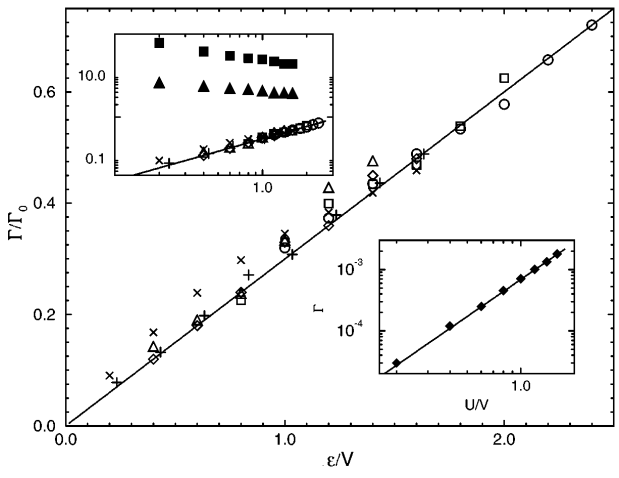

FIG. 2. Same as Fig. 1 in 3D. DD data at $U/V = 1.2$ and $W/V = 4$ with $L = 4$ (○), $L = 5$ (□), $L = 6$ (◇), and $L = 7$ (△). FGR data: $W/V = 4$ with $L = 10$ (×); $W/V = 2$ with $L = 8$ (+). Here $C = 0.3$. Upper inset: the same on a log-log scale with FGR data at higher disorders [$W/V = 12$ (▲) and $W/V = 20$ (■) ($L = 10$)]. Lower inset: DD data for Γ vs U/V at $W/V = 4, L = 6, V = \epsilon = 0.5$ (solid line: $\Gamma = 0.3\Gamma_0$).

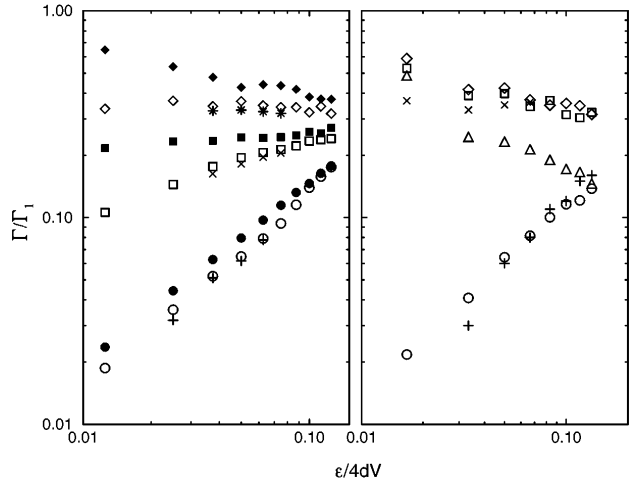

FIG. 3. Energy dependence of the rescaled Breit-Wigner width Γ/Γ_1 in 2D (left) and 3D (right). FGR data in 2D: $W/V = 2$ with $L = 20$ (○) and $L = 30$ (●); $W/V = 4$ with $L = 20$ (□) and $L = 30$ (■); $W/V = 6$ with $L = 20$ (◇) and $L = 30$ (◆). DD data in 2D at $L = 20$, $U/V = 0.6$: $W/V = 2$ (+), $W/V = 4$ (×), and $W/V = 6$ (∗). FGR data in 3D at $L = 10$: $W/V = 4$ (○), $W/V = 12$ (□), $W/V = 20$ (◇), and $W/V = 28$ (△). DD data in 3D at $L = 6$, $U/V = 1.2$: $W/V = 4$ (+) and $W/V = 12$ (×).

block, and the scaling $\Gamma \propto L^{-d}$ is not valid any more. In the limit $1 < l_1 \ll L$, it is natural to expect another scaling $\Gamma \propto l_1^{-d}$. To check this scaling we computed the inverse participation ratio $\xi \sim l_1^d$, which allowed us to calculate the ergodic value $\Gamma_1 = U^2/V\xi$.

At a sufficiently high excitation energy, the real width should be $\Gamma \sim \Gamma_1$ which gives the correct scaling with the system size in the localized regime according to the numerical data. This would explain why, in a block of fixed size, Γ increases with increasing disorder (see insets in Figs. 1 and 2). While this estimate gives the correct value of Γ at high energies, i.e., $\epsilon \approx 2V$ (Fig. 3), it does not explain the change of energy dependence with disorder. We should note that even in this unusual regime both the direct diagonalization and the Fermi golden rule computations give the same value of the width Γ.

It is clear that the change of the energy dependence of Γ cannot be explained in the framework of the ergodic transition matrix elements $U_s^2 \sim (U/V)^2\Delta^3/V$, where $\Delta \sim V/L^d$ is the one-particle level spacing in a block of size L. At the same time, the numerical results for the two-particle density of states ρ_2 definitely show that it increases linearly with the excitation energy ϵ 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 [13–15], it is known that the diffusive nature of the dynamics should be taken into account. For an excitation energy ϵ much bigger than the Thouless energy E_c, the quasiparticle decay rate is $\Gamma_D \sim U_s^2\rho_3 \sim \Delta(U\epsilon/VE_c)^{d/2}$, where $\rho_3 \sim \rho_2\epsilon/\Delta$ 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, $\Delta < \epsilon \ll E_c$, this rate is $\Gamma_D \sim \Delta(U\epsilon/VE_c)^2$ [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 [16]. The different nonergodic regimes can be described by the following approximate expression [17]:

$$U_s^2 \sim \left(\frac{U}{V}\right)^2 \frac{\Delta^2}{g^2}\left(1 + \frac{\epsilon}{E_c}\right)^{d/2-2}, \qquad (4)$$

where $g = E_c/\Delta$ is the conductance, assumed to be much bigger than one. According to (4) the TIQ width $\Gamma \sim U_s^2\rho_2$ 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. The energy dependence, $\Gamma \propto \epsilon^{d/2-1}$, from (4) is in agreement with the numerical data for $d = 2$ (Fig. 3), but in 3D the data indicate an algebraic dependence with the power $\alpha < 0$ ($\alpha \approx -0.2$ for $W = 12V$ and $\alpha \approx -0.3$ for $W = 20V$) instead of the theoretical value $\alpha = 1/2$. There could be different reasons for this discrepancy. One case, $W = 20V$, corresponds to the localized regime while the theory requires a metallic behavior. The other case, $W = 12V$, even though still delocalized, is quite close to the critical value W_c. Our data indicate that, in the metallic regime with $2 < W/V < 12$, the power α smoothly changes from 1 to -0.2.

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 $l_1 \gg 1$. 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 $E_c \approx \Delta \sim V/l_1^d$. This gives $\Gamma \sim \Gamma_1(\epsilon/\Delta)^\alpha$, where α 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 ϵ_{m2} is defined by the condition $\kappa = \Gamma\rho_c > 1$ [1,2]. Since $\rho_c \sim \epsilon/\Delta^2$, the above expressions for Γ give

$$\epsilon_{m2} \sim \frac{V}{l_1^d}\left(\frac{V}{U}\right)^{2/(1+\alpha)} \sim V\left(\frac{\epsilon_{m1}}{V}\right)^{\nu d}\left(\frac{V}{U}\right)^{2/(1+\alpha)}, \qquad (5)$$

where $\epsilon_{m1} \sim Vl_1^{-1/\nu}$ is the one-particle mobility edge. The one-particle critical exponent is $\nu \approx 1.5$ [18]. Because of this, for $U \sim V$, the edge $\epsilon_{m2} \ll \epsilon_{m1}$. The above result (5) gives a much smaller value for ϵ_{m2} than the one given by the Imry estimate [2]. 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 [2]. The condition that the TIQ delocalization border in U at $\epsilon \sim V$ is the same as for TIP ($U > V/l_1^{d/2}$ [1,2]) gives $\alpha = 0$.

The numerical results for the dependence of $\kappa = \Gamma\rho_c$ on ϵ are presented in Fig. 4. To determine numerically

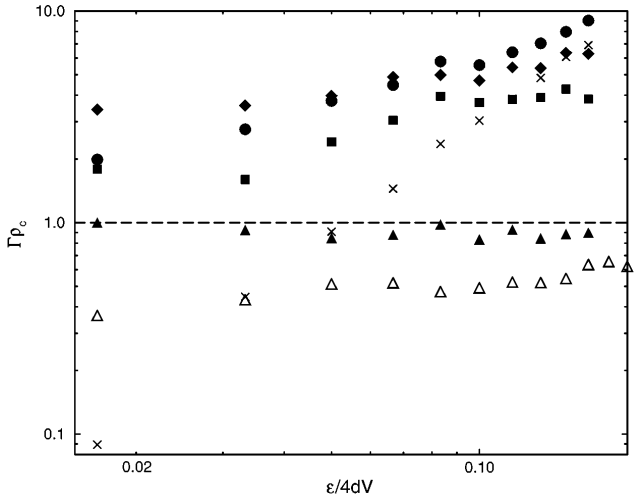

FIG. 4. Energy dependence of the TIQ delocalization parameter $\kappa = \Gamma\rho_c$ in 3D (FGR data) at $U/V = 1.2$: $L = 7$ for $W/V = 28$ (△); $L = 10$ for $W/V = 4$ (×), $W/V = 12$ (●), $W/V = 16.8$ (■), $W/V = 10$ (◆), and $W/V = 28$ (▲). The dashed line shows the TIQ mobility edge $\kappa = \Gamma\rho_c = 1$.

the density of coupled states $\rho_c \sim \epsilon l_1^{2D}/V^2$ in the localized regime, we computed it by taking into account only those TIQ states which give contributions larger than 30% of the value of Γ (the data were not sensitive to the cutoff value). The density ρ_c defined in this way is independent of the system size when $L > l_1$. The data show that for $W = 28V$ 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 κ 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 ϵ_{m2}.

In our consideration, all inelastic processes involving hole excitations have been suppressed so that $\Gamma_D = 0$. This is a crucial assumption. Apparently, for $\epsilon \gg \Delta$ there is no good reason to assume that $\Gamma_D \ll \Gamma$ since there $\Gamma_D/\Gamma \sim \rho_3/\rho_2 \sim \epsilon/\Delta \gg 1$. However, for $\epsilon \sim \Delta \sim V/l_1^d$, this estimate gives $\Gamma_D \sim \Gamma$. In addition to that, at $\epsilon \sim \Delta$ the decay rate Γ_D should be strongly suppressed since energetically it is not possible to excite many holes in a block of size l_1 [2] with a discrete spectrum. Also, according to the recent results [19], in a quantum dot $\Gamma_D = 0$ for energy $\epsilon < \epsilon_1 \sim \Delta\sqrt{g}$ and $U \sim V$. For a dot (block) of size l_1 this gives $\epsilon_1 \sim \Delta$. Thus it is possible that, for $U \sim V$ slightly above the mobility edge (5), $\epsilon_{m2} \sim \Delta$, the propagation of the TIQ pairs through the lattice (transitions between different blocks) will not be strongly affected by the inelastic processes of hole excitation neglected in our model. Besides that, $\epsilon_{m2} \sim \Delta$ is the minimum possible mobility edge in our model with the frozen Fermi sea. This indicates a possibility of interaction-induced rearrangement of the ground state from the localized to conducting phase. Energetically, the delocalization of TIP pairs causes a decrease of the kinetic energy by $\delta E_- \sim \delta p \sim V/l_1$, which can be larger than the energy increase due to the interaction $\delta E_+ \sim U/l_1^d$. The above results could give a hint as to an explanation of recent experiments on the interaction-induced metal-insulator transition in 2D disordered systems [20].

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