Three-dimensional Anderson transition for two electrons in two dimensions

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(Received 17 February 1999; revised manuscript received 23 August 1999)

It is shown that Coulomb interaction can lead to the delocalization of two-electron states in a two-dimensional disordered potential in a way similar to the Anderson transition in three dimensions. At a fixed disorder strength the localized phase corresponds to a low electron density and a large value of the parameter r_s. Analytical results are supported by a numerical study of level spacing statistics.

Contrary to a well-established theoretical result,[1] according to which noninteracting electrons are always localized in a two-dimensional (2D) disordered potential, the pioneering experiment by Kravchenko *et al.*[2] demonstrated the existence of metal-insulator transition for real interacting electrons in two dimensions. The ensemble of experimental data obtained by different groups[3–8] clearly indicates the important role played by interaction. In the majority of experiments the Coulomb energy of electron-electron interaction E_{ee} is significantly larger than the Fermi energy E_F estimated for noninteracting electron gas in the absence of disorder. The ratio of these energies is characterized by the dimensionless parameter $r_s=1/\sqrt{\pi n_s}a_B^*\simeq E_{ee}/E_F$, where n_s is the electron density in two dimensions, and $a_B^*=\hbar^2\epsilon_0/m^*e^2, m^*$, and ϵ_0 are the effective Bohr radius, electron mass, and dielectric constant respectively. Such large r_s values as 10–30 have been reached experimentally.[2–8] At these r_s values the electrons are located far from each other, and it is natural to assume that in this regime the interaction effects will be dominated by pair interaction. The important role of the residual two-body interaction is also clear from the fact that in the Hartree-Fock (mean field) approximation the problem is again reduced to a one-particle 2D disordered potential with localized eigenstates.[1]

The problem of two electrons interacting in the localized phase is rather nontrivial. Indeed, recently it has been shown that a short-range repulsive/attractive interaction between two particles can destroy one-particle localization and lead to the creation of pairs propagating at a distance much larger than their size.[9–13] The pair size is of the order of the one-particle localization length l_1. Inside this length the collisions between particles destroy the quantum interference that results in their coherent propagation at a distance $l_c \gg l_1$. The important point is that only pairs can propagate at a large distance. Indeed, the particles separated by a distance $R \gg l_1$ have an exponentially small overlap; the interaction between them is weak, and such states are localized as in the noninteracting case. According to the theoretical estimates[9,10,13] in two dimensions the localization length l_c grows exponentially with l_1 according to the relation $\ln(l_c/l_1)\sim\kappa>1$. Here $\kappa\sim\Gamma_2\rho_2$, where $\Gamma_2\sim U^2/(Vl_1^2)$ is the interaction-induced transition rate between localized states in, e.g., the 2D Anderson model, $\rho_2\sim l_1^4/V$ is the density of two-particle states directly coupled by interaction, V is the hopping between nearest sites, U is the on-site (nearest) interaction, and the energy is taken in the middle of the band. In a sense the above estimate is similar to the case of one-particle localization in two dimensions, where $\ln l_1\sim k_F l \sim (V/W)^2$, and the product of the Fermi wave vector k_F on a mean free path l is proportional to a local diffusion rate[14]; W is the strength of the on-site disorder. Indeed, in the same manner the interaction-induced diffusion rate of a pair is given by $D_2\sim l_1^2\Gamma_2\sim\kappa/l_1^2\propto\ln l_c$. According to the above estimates l_c should vary smoothly with the effective interaction strength characterized by the dimensionless parameter κ. However, this consideration is valid only for a short-range interaction, while the analysis of the long-range Coulomb interaction requires a separate study. The investigation of this case is also dictated by the experiments,[2–8] where the electrons are not screened and are located far from each other ($r_s\gg 1$). On qualitative grounds one can expect that the effect of Coulomb interaction will be stronger since electrons are always interacting differently from the case of short-range interaction. As we will see below, the interaction effects will play an important role even at low density when the electrons are far from each other ($R\gg l_1$), and where the Coulomb interaction can lead to a delocalization transition similar to one in the 3D Anderson model. It is convenient to study this transition by means of level spacing statistics, as was done for the 3D one-particle case in Ref. 15.

To analyze the effect of the Coulomb interaction between two electrons, let us consider a 2D Anderson model with diagonal disorder ($-W/2<E_i<W/2$), hopping V, lattice constant $a=1$, and interaction $U/|\mathbf{r}_1-\mathbf{r}_2|$. In these notations $r_s=U/(2V\sqrt{\pi n_s})$, and it is convenient to introduce another dimensionless parameter $r_L=Ul_1/2\sqrt{\pi}V$, which is equal to r_s at $n_s=1/l_1^2$. We will consider the case with $U\sim V$ and $r_s\gg 1$ when the average distance between electrons $R=|\mathbf{r}_1-\mathbf{r}_2|$ is much larger than their noninteracting localization length: $R\sim 1/\sqrt{n_s}\sim r_s\gg l_1\gg 1$. In this case the two-body interelectron interaction has a dipole-dipole form, and is of the order of $U_{dd}\sim U\Delta\mathbf{r}_1\Delta\mathbf{r}_2/R^3\sim Ul_1^2/R^3$. Indeed, the first two terms in the expansion of the Coulomb interaction give only mean-field corrections to the one-particle potential, and the nontrivial two-body term appears only in second order in the electron displacements $\Delta\mathbf{r}_1\sim\Delta\mathbf{r}_2\sim l_1$ near their initial positions $\mathbf{r}_{1,2}$. The matrix element of this dipole-dipole interaction between localized noninteracting eigenstates is of the order of $U_s\sim U\Sigma\Delta\mathbf{r}_1\Delta\mathbf{r}_2\psi^4/R^3\sim U/R^3$. Here $\psi\sim\exp$

$(-|\Delta \mathbf{r}_{1,2}|/l_1)/l_1$ are localized one-electron states, and due to localization the sum runs over l_1^4 sites and each term in the sum has a random sign. According to the Fermi golden rule these matrix elements give the interaction-induced transition rate $\Gamma_e \sim U_s^2 \rho_2 \sim U_{dd}^2/V$, where the density of coupled states in the middle of the energy band is still $\rho_2 \sim l_1^4/V$, since, due to localization, only jumps on a distance l_1 are allowed. These interaction-induced matrix elements mix two-electron states if $\kappa_e \sim \Gamma_e \rho_2 > 1$, that corresponds to $R < l_1 (U l_1/V)^{1/3}$ [a similar estimate for electrons in three dimensions was given in Ref. 9(b)]. Since $l_1 \gg 1$, the condition $R \gg l_1$ is still satisfied. For $\kappa_e > 1$ these transitions lead to a diffusion with the rate

$$D_e \sim l_1^2 \Gamma_e \sim V \kappa_e / l_1^2. \tag{1}$$

This diffusion expands in an effective 3D space. Indeed, the center of mass of two electrons diffuses in a 2D lattice plane, and in addition the electrons diffusively rotate on a ring of radius R and width l_1. The radius of the ring is related to the e-e energy $E \sim U/R$, which remains constant. Since $R \gg l_1$ it takes a long time to make one rotation along the ring. As for the 3D Anderson model, this diffusion becomes delocalized when the hopping is larger than the level spacing between directly coupled states, namely,

$$\chi_e \sim \kappa_e^{1/6} \sim r_L^{4/3}/r_s > 1. \tag{2}$$

Formally the situation corresponds to a quasi-two-dimensional case with $M_{ef} \approx \pi R/l_1 = \pi r_L^{1/3} >> 1$ parallel planes (the number of circles of size l_1 in the ring), so that the pair localization length l_c jumps from $l_c \sim l_1$ for $\kappa_e < 1$ to $l_c \sim l_1 \exp(\pi \kappa_e r_L^{1/3}) \gg l_1$ above the transition $\kappa_e > 1$. The transition is sharp and similar to a 3D Anderson transition, when $r_s > r_L \gg 1$. Indeed, according to the standard scaling arguments[14] for a quasi-2D Anderson model with M coupled planes and isotropic hopping, the localization length jumps from $l_1 \sim 1$ to $l_1 \sim \exp(g)$ when W crosses the 3D critical point W_c. Here $g \sim M(W_c/W)^2$ is the conductance equal to the ratio of Thouless energy E_c to level spacing Δ. In a similar way, for the case of two electrons we can write that $E_c \sim D_e/L^2$, where L is the system size in which the center of mass moves diffusively with the rate D_e. Since for each position of the first electron, or the center of mass, the second electron can occupy approximately $l_1^2 M_{ef}$ states, then the level spacing is $\Delta \sim V/(L^2 l_1^2 M_{ef})$ and the effective conductance is $g_{ef} \sim E_c/\Delta \sim D_e l_1^2 M_{ef}/V \sim \kappa_e M_{ef}$. As the result above the transition $l_c/l_1 \sim \exp(g_{ef}) \sim \exp(\kappa_e M_{ef})$, in agreement with the estimate given above. If electrons would be able to move inside the ring then M_{ef} would be even larger ($M_{ef} \sim r_L^{2/3}$).

It is important to stress that the parameter χ_e, which determines the delocalization border and measures the effective strength of two-body interaction, decreases with the increase of r_s. This looks to be against the common lore, according to which the larger r_s is, the stronger the e-e-interaction is. The reason for this contradiction with Eq. (2) is simply due to the fact that r_s compares E_{ee} with E_F computed in the *absence* of disorder. In the presence of not very weak disorder ($r_D = E_{ee}/W \ll 1$ and $r_L \gg 1$), one-electron states are localized and form the basis of Coulomb glass.[16] In this Coulomb glass phase the $e-e$-interaction becomes weaker and weaker with the growth of the average distance between electrons $R \sim n_s^{-1/2} \propto r_s$, in natural agreement with Eq. (2). Transition border (2) was obtained for excited states. However, it is clear that if the interaction is not able to delocalize the excited states then the low-energy states will also remain localized, since the two-electron density ρ_2 drops at low energy. In this sense Eq. (2) determines the upper border for r_s.

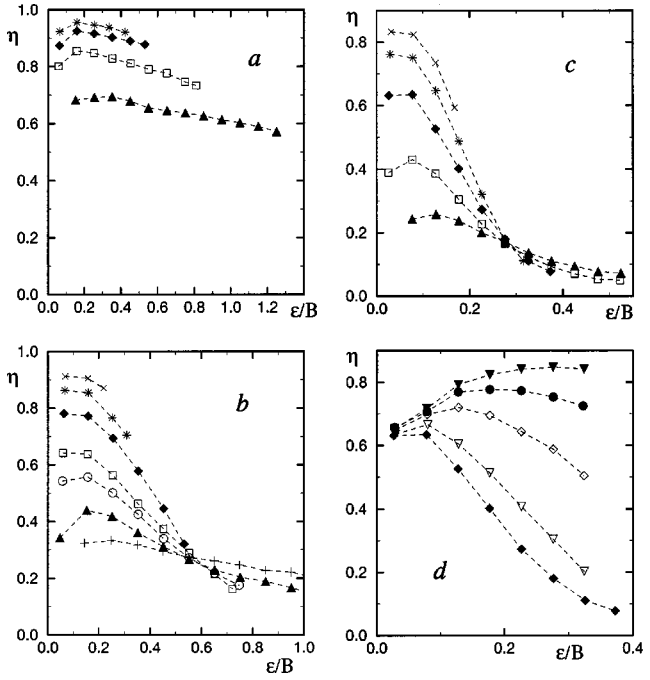

FIG. 1. Dependence of η on the rescaled one-electron energy ϵ/B (with $B=4V$) for different W, system size L[(a–c)] and interaction strength U(d). For (a)–(c), the sizes are $L=6$ (+),8 (full triangle); 10 (o); 12 (□); 16 (full diamond), 20 (*), and 24 (×), so that $2.39 \leqslant r_s \leqslant 9.57$, $U/V=2$, and $W/V=15$(a),10(b), and 7(c). For (d), $W/V=7$, $L=16$, and $U/V=2$ (full diamond), 1(▽),0.4(◇), 0.2 (full circle), and 0.1 (full trangle).

To study delocalization transition (2), the level spacing statistics $P(s)$ is determined numerically for different system sizes L. To follow the transition from the localized phase with the Poisson statistics $P_P(s)$ to the delocalized phase with the Wigner-Dyson statistics $P_{WD}(s)$, it is convenient to use the parameter $\eta = \int_0^{s_0} [P(s) - P_{WD}(s)]ds / \int_0^{s_0} [P_P(s) - P_{WD}(s)]ds$, where $s_0 = 0.4729\ldots$ is the intersection point of $P_P(s)$ and $P_{WD}(s)$. In this way $\eta=1$ corresponds to the Poissonian case, and $\eta=0$ to $P_{WD}(s)$. The dependence of η on the one-electron energy $\epsilon = E/2$, counted from the ground state, is shown in Fig. 1 for different disorder W and interaction strength U. Usually $ND=4000$ realizations of disorder are used to compute $P(s)$ for each spacing between levels i and $i+1$, counted from the ground state. Then these $P(s)$'s are averaged in a small energy interval that allows one to increase the total statistics for final $P(s)$ and η from $NS=12\,000$ for low-energy states up to $NS=10^6$ at high energies with a larger density of levels. In Fig. 1 the size of the energy interval is equal to the distance between symbols. The matrix diagonalization is done in the one-electron eigenbasis truncated at high energies, that allows one to study

two-electron low-energy excitations (with energy E) at large system sizes $L \leqslant 24$. The periodic boundary conditions are used for one-electron states, and the Coulomb interaction is taken between electrons in one cell of size L and with a charge of eight images in eight nearby cells. Coulomb interaction periodic in one cell gave similar results. Only the triplet case was considered, but the singlet case should give similar results.[9,12]

The results of Fig. 1(a) show that at fixed interaction and strong disorder $W/V=15$ the $P(s)$ statistics approaches the Poisson distribution ($\eta=1$) at large system size L and large $r_s=UL/(2\sqrt{2\pi}V)$. This means that all states are localized. For smaller disorder the situation becomes different [Figs. 1(b) and 1(c)]. While near the ground state $\eta \to 1$ still holds for large L, the tendency is inverted above some critical energy ϵ_c where $\eta \to 0$. All curves $\eta(\epsilon)$ for different L's are crossed in one point in a way similar to the 3D Anderson transition studied in Ref. 15.

This result can be understood in the following way. At a strong Coulomb interaction $U \sim V$ the excitation energy ϵ is related to the distance between electrons R: $\epsilon \sim U/R$ (a similar relation was used in Ref. 16 for the Coulomb glass). At higher ϵ the distance R becomes smaller, the interaction is stronger, and for $\epsilon > \epsilon_c$ the delocalization border $R \sim U/\epsilon \sim l_1 r_L^{1/3}$ [Eq. (2)] is crossed and the states become delocalized. Since the distance R is related to the two-electron energy $E=2\epsilon \sim U/R$, the spacing statistics $P(s)$, which is local in energy and therefore also in R, is not influenced by states where particles are far from each other. In this sense the situation is different from the case of short-range interaction. According to the above arguments $\tilde{\epsilon}_c=\epsilon_c l_1^{4/3}/B$ should remain constant when l_1 changes with disorder. The value of l_1 can be extracted from the average inverse participation ratio $\xi_1=1/\Sigma|\psi|^4$ computed for one-particle states in the middle of the band ($l_1 \sim \sqrt{\xi_1}$). For $L=24$ and $W/V=10$, 7, and 5, we have $\xi_1=11.6$, 36.7, and 84.2, respectively, which, with $\epsilon_c/B \approx 0.6$, 0.28, and 0.16 (the case $W/V=5$ is not shown), gives $\tilde{\epsilon}_c=3.08 \pm 0.01$, in satisfactory agreement with the above expectations. The variation of η with the interaction U is shown in Fig. 1(d). According to this η increases with the decrease of U (states become more localized) in agreement with the general estimate (2). The analysis above allows to understand the dependence of η on ϵ and L. Another reason for the decrease of η at higher ϵ is related to the fact that the two-electron density of states ρ_2 grows with energy, which allows us to mix levels more easily. A more detailed theory should take this fact into account and also analyze the variation of the rate Γ with ϵ. The results in this direction will be published elsewhere.[17]

The $P(s)$ statistics for two electrons in two-dimensions near the critical point ϵ_c/B is shown in Fig. 2. Its comparison with the critical statistics in the 3D Anderson model, taken from Ref. 18 (see also Ref. 19), demonstrates that both statistics are really in very close agreement with the arguments given above. At the critical point the value of η_c is close to its value in the Anderson model ($\eta_c=0.20$). The small deviations from this value in the case of 2D electrons [$\eta_c \approx 0.25 (W/V=10)$ and $0.17 (W/V=7)$] can be attributed

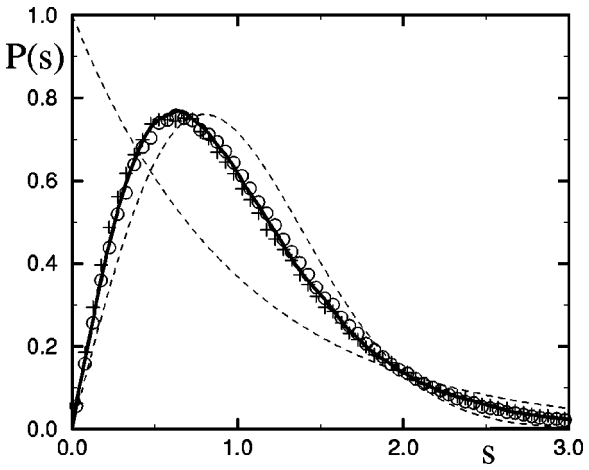

FIG. 2. Level statistics $P(s)$ for two 2D electrons at the critical point: (+)—$W/V=10$, $L=12 (0.55 \leqslant \epsilon/B \leqslant 0.65)$, and total statistics $NS=4\times10^5$ [see Fig. 1(b)]. (o)—$W/V=7$, $L=16 (0.25 \leqslant \epsilon/B \leqslant 0.3)$, and $NS=5\times10^5$ [see Fig. 1(c)]. The full line shows the critical $P(s)$ in the 3D Anderson model ($W/V=16.5$ and $L=14$, taken from Ref. 18); the dashed lines give Poisson statistics and the Wigner surmise.

to the fact that the parameter $l_1^{1/3}$ was not sufficiently large. The investigation of the case with larger l_1 requires a significant increase of the system size $L>24$. Indeed, for $L=24$ and $W/V=5$ the localization length becomes comparable with $L (l_1 \sim \sqrt{\xi_1} \approx 9)$, which gives a decrease of $\eta_c \approx 0.13$.

Of course, one cannot expect that the simple model of two electrons considered above will explain the variety of experimental results obtained by different groups.[3–8] However, it shows some tendencies which are in agreement with the experiment. Indeed at large r_s (a density lower than some critical n_c), experiments demonstrate the transition from a metal to an insulator. According to Fig. 4 in Ref. 6, the density at the transition $n_c \propto 1/\sqrt{r_s}$ drops exponentially with the increase or decrease of the mobility or disorder $\mu \propto 1/W^2$. This agrees qualitatively with estimate (2) according to which near the transition $\ln n_c \sim \ln(1/r_s) \sim -\ln r_L \sim -1/W^2$. However, the condition $r_s \gg r_L$ seems not to be well satisfied, and apparently multielectron effects should also be taken into account. Another interesting experimental result (Fig. 2 in Ref. 8) shows that the conductivity σ_c near the critical point grows with an increase of density n_c or disorder W. This is in qualitative agreement with estimate (1) according to which $\sigma_c \sim D_e/V \sim 1/l_1^2 \propto r_L^{-2} \propto r_s^{-8/3} \propto n_c^{4/3}$ since near the critical point [Eq. (2)] $\kappa_e \sim 1$ and $r_s \sim r_L^{4/3}$. It is also interesting to remark that the scaling index $\nu \approx 1.5$ found in Ref. 3 is close to the index $\nu \approx 1.5$ near the 3D Anderson transition (the fact that in three dimensions $\nu \approx s$ can be related to the observed symmetry of the I-V curves). Finally, let us note that recent results[20] also show a delocalization effect of the interaction for highly excited states in two dimensions.

I thank Y. Hanein and A. Hamilton for the stimulating discussions of experimental results, D. Braun for the possibility to use the data of Ref. 18, and K. Frahm for a useful suggestion.

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