Transmission of two interacting electrons

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Abstract

The transmission of two electrons through a region where they interact is found to be enhanced by a renormalization of the repulsive interaction. For a specific example of the single-particle Hamiltonian, which includes a strongly attractive potential, the renormalized interaction becomes attractive, and the transmission has a pronounced maximum as function of the depth of the single-electron attractive potential. The results apply directly to a simple model of scattering of two interacting electrons by a quantum dot.

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Transport through quantum dots, systems of quantum dots, or one-dimensional wires is currently the subject of much interest. Such structures have potential applications as artificial atomic or molecular devices, and are very instrumental in studying strong correlations and their implications, e.g., the Kondo effect or magnetic transitions. The theoretical studies of the transmission through such systems concentrate mostly on the single-electron conductance, with the electron-electron interaction taken into account in an approximate manner, e.g., via the charging energy (introducing the notion of the dot capacitance) or by using the slave–boson mean–field approximation. Exact solutions of interacting electrons, in this context, focus mainly on the electronic spectrum of two electrons, confined to a restricted region in space, which models the quantum dot (see, e.g., Ref. ). Obviously, two is the minimal number of electrons required to study interactions. However, devices including two electrons can be investigated experimentally, and may have potential applications in quantum computers. Recently, we have studied the electronic spectrum of two interacting electrons on artificial atoms, and found that the understanding of the full physical behavior of such systems requires a consideration of the entire system, including the leads. In that calculation we found that interactions can delocalize one of the electrons, depending on the strength of the connections between the dot and the leads. In other words, it is not sufficient to treat the interacting region as an isolated system. This transition of an electron from the bound state into the band may be relevant for the metal-insulator transition brought about by donor ionization. The exact solution of the two electron problem yields a renormalized value of the interaction, which depends on the energy.

In this paper we study the one-dimensional transmission of two electrons, when they interact via a contact potential at a certain point. We consider the Hamiltonian

\[
\mathcal{H}(x_1, \sigma_1, x_2, \sigma_2) = \mathcal{H}_0(x_1, x_2) + U\delta(x_1)\delta(x_2)\delta_{\sigma_1, -\sigma_2},
\]

\[
\mathcal{H}_0(x_1, x_2) = \mathcal{H}_{sp}(x_1) + \mathcal{H}_{sp}(x_2),
\]

(1)

where \(x_i\) and \(\sigma_i\) are the coordinate and the spin component of the \(i\)th electron, and \(\mathcal{H}_{sp}\) is
the single–particle Hamiltonian, independent of the spin components. In (1), $U$ is the local
(Hubbard) interaction. This is a continuum version of the Anderson impurity model. Since $H_0$
does not depend on the spins, and since the interaction vanishes on the triplet states (which are antisymmetric in space and vanish when $x_1 = x_2 = 0$), it is convenient to separate the Hilbert space into triplet and singlet states. The former are unaffected by the interaction, and their scattering is fully described by the single–electron non–interacting transmission. The rest of this paper is devoted to an exact solution of the singlet case. We express the scattered wave function in terms of the single–particle spectrum, and calculate the two–electron current.

Our explicit calculations are carried out for a single–particle Hamiltonian which has an attractive short-range potential, resulting with a bound state, whose inverse localization length $\kappa$ determines the electric current (or equivalently the transmission) in the absence of the interaction. When one views the model as a ‘quantum dot’ coupled to ideal one–dimensional conductors (‘leads’), then the strength of the attractive single–particle potential can be regarded as the gate voltage applied to the ‘dot’.

We consider explicitly two scenarios for the transmitted current. In the first case, the incident wave contains two propagating electrons (with wave numbers $p_1$ and $p_2$). For our contact interaction [Eq. (1)], we show that in this case there is no effect of the interaction: for a sample of large length $L$, the current is given by

$$ j = e(p_1|t_{p_1}|^2 + p_2|t_{p_2}|^2)/(mL) + O(U/L^2), $$

(2)

where $t_p$ is the single–electron non–interacting transmission amplitude. The reason for this simple behavior is quite clear: In our model, the two electrons “feel” one another only when both are at $x = 0$, and the amplitude for this to occur is proportional to $1/L$.

In the second case, the “impinging” wave contains one propagating electron (with wave number $p$), while the other is captured by the attractive potential. Now the current is found to have the form

$$ j = epT(U, p)/(mL), $$

(3)

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and the effective transmission $T(U,p)$ has a very interesting dependence on the single-electron parameters and on $U$. Specifically, Fig. 1 shows the dependence of $T(U,p)$ on $\kappa$, for several values of $U$ and $p$ (in units of $\hbar^2/(2m)$ and of the large wave number cutoff $\omega$, respectively). Clearly, $T(U,p)$ increases significantly when $U > 0$ (compared to the case $U = 0$), reflecting the “screening” of the attractive single-electron potential by the bound electron, eventually leading to a transition from the doubly bound ‘insulating’ state to a state in which one electron is ‘free’, which can be called ‘metallic’. [12] For the special $\delta$–function attractive potential discussed below, and for large $\kappa$, the arguments of Ref. [12] imply that this transition happens for $U > 2$. Indeed, when $U < 2$ Fig. 1 (left panels) shows a monotonic decrease in $T$, but $T$ is much larger than the non–interacting result. At $U = 2$ (central panels), $T$ is found to approach a finite plateau value even at large $\kappa$. This value increases with $p$. For $U > 2$, we observe a peak in $T$, which moves to larger values of $\kappa$ as $U$ approaches 2 from above. This peak has $T \approx 1$ for small $p$, but it decreases and broadens as $p$ increases. As we show below, this peak corresponds to the resonance with the just-bound doubly-occupied state. $T(U,p)$ decreases for larger $\kappa$, when the effective renormalized interaction becomes more and more attractive.

In addition to the above peak (and to the peak at $\kappa = 0$), we sometimes find a third peak at $p \approx \kappa \ll \omega$, i. e. when the total energy of the two electrons vanishes; at larger $\kappa$’s the incoming electron is no longer able to ‘ionize’ the bound electron (see e. g. $T(4,.1)$). At this point, both the product of the transmitted and reflected wave functions and the product of the ‘bound’ and ‘free’ electron wave functions on the ‘dot’ are maximal, giving a peak in the interaction between the free and the bound electron and therefore in the screening. This peak disappears as $p$ increases. The peaked structure of the transmission versus $\kappa$, which represents the peaks of $T$ as function of the gate voltage on the ‘dot’, is very different from that found in the naive Coulomb blockade picture. [4] In the latter case, the distances between peaks would be equal to $U$! We conclude that this naive picture fails for our exactly solved example.

We now give more technical details. We consider only the singlet scattering wave func-
tions, which are spatially symmetric, \( \Psi(x_1, x_2) = \Psi(x_2, x_1) \). At total energy \( E \), we split \( \Psi \) into \( \Psi = \Psi_0 + \Psi_S \), where \( \Psi_0 \) is the ‘incoming’ solution of \( \mathcal{H}_0 \), with the same energy \( E^+ \equiv (E + i\eta) \) (with \( \eta \to 0^+ \)), \( (\mathcal{H}_0 - E^+)\Psi_0 = 0 \). It then follows that

\[
\Psi_S(x_1, x_2) = U G_E(x_1, x_2; 0, 0) \Psi_0(0, 0),
\]

(4)

where \( G_E \) is the two–particle Green’s function of the interacting Hamiltonian, obeying

\[
(\mathcal{H} - E^+)G_E(x_1, x_2; x'_1, x'_2) = -\delta(x_1 - x'_1)\delta(x_2 - x'_2). \tag{5}
\]

For the model Hamiltonian given by (1) one can express \( G_E \) in terms of the two–particle Green’s function of the non–interacting system, \( G^0_E \):

\[
(\mathcal{H}_0 - E^+)G^0_E(x_1, x_2; x'_1, x'_2) = -\delta(x_1 - x'_1)\delta(x_2 - x'_2). \tag{6}
\]

Combining Eqs. (5) and (6) yields

\[
G_E(x_1, x_2; x'_1, x'_2) = G^0_E(x_1, x_2; x'_1, x'_2) + U G^0_E(0, 0; x'_1, x'_2)G_E(x_1, x_2; 0, 0), \tag{7}
\]

and hence

\[
G_E(x_1, x_2; 0, 0) = G^0_E(x_1, x_2; 0, 0)/[1 - U G^0_E(0, 0; 0, 0)] \equiv F_E G^0_E(x_1, x_2; 0, 0)/U. \tag{8}
\]

This immediately yields \( G_E(x_1, x_2; x'_1, x'_2) \) and

\[
\Psi(x_1, x_2) = \Psi_0(x_1, x_2) + F_E G^0_E(x_1, x_2; 0, 0)\Psi_0(0, 0). \tag{9}
\]

The right hand side of (8) is determined solely by the eigenstates of the non–interacting Hamiltonian \( \mathcal{H}_0 \). \( U \) appears only in the form \( F_E \), which turns out to be quite important in determining the transmission characteristics.

Instead of solving directly for the two–electron non–interacting Green’s function \( G^0_E \), we present this function in terms of the single–particle Green’s function, \( g_\epsilon(x, x') \), of \( \mathcal{H}_{sp} \),

\[
(\mathcal{H}_{sp}(x) - \epsilon^+)g_\epsilon(x, x') = -\delta(x - x'), \tag{10}
\]

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where $\epsilon^+ = \epsilon + i\eta$, and $\eta \to 0^+$. $g_\epsilon(x, x')$ can also be written in terms of its spectral decomposition,

$$g_\epsilon(x, x') = \sum_n \frac{\phi_n(x)\phi^*_n(x')}{\epsilon^+ - \epsilon_n}, \quad (11)$$

where $\mathcal{H}_{sp}\phi_n = \epsilon_n\phi_n$. Writing the non–interacting singlet spatial wave functions as

$$\Psi^0_{nm}(x_1, x_2) = \left(\phi_n(x_1)\phi_m(x_2) + \phi_n(x_2)\phi_m(x_1)\right)/\sqrt{2(n+\delta_{nm})}, \quad (12)$$

with energy $E(n, m) = \epsilon_n + \epsilon_m$, one can show that the spectral decomposition of the singlet non–interacting two–particle Green’s function is

$$G^0_{E}(x_1, x_2; x'_1, x'_2) = \sum_{nm} \frac{\phi_n(x_1)\phi_m(x_2)\phi^*_n(x'_1)\phi^*_m(x'_2)}{E^+ - \epsilon_n - \epsilon_m}. \quad (13)$$

Using the two spectral representations, we obtain

$$G^0_{E}(x_1, x_2; x'_1, x'_2) = -\frac{1}{\pi} \int_{-\infty}^{\infty} d\epsilon \ g_{E-\epsilon}(x_1, x'_1) \Im g_\epsilon(x_2, x'_2) =$$

$$\frac{i}{2\pi} \int_{-\infty}^{\infty} d\epsilon \ g_{E-\epsilon}(x_1, x'_1) g_\epsilon(x_2, x'_2), \quad (14)$$

where the last equality follows from the Kramers–Kronig relations.

We next calculate the quantum average of the current density operator at $x = x_0$, in the exact singlet state $\Psi$. Noting that $\Psi(x_1, x_2)$ is symmetric in $x_1, x_2$, this average is

$$j(x_0) = \frac{2e\hbar}{m} \Im \int dx_1 dx_2 \delta(x_1 - x_0) \Psi^*(x_1, x_2) \frac{d}{dx_1} \Psi(x_1, x_2), \quad (15)$$

where $\Psi$ is given by Eq. (12). The explicit calculation of $j$ now requires only integrals involving the non–interacting functions $\Psi^0(x_1, x_2)$ and $g_\epsilon(x, 0)$. In what follows, we shall assume that $\Psi^0 \equiv \Psi_{pq}^0$, as given by Eq. (12), and that the total energy is given by $E = \epsilon_p + \epsilon_q$. The calculation is then facilitated using identities such as

$$\int dx \phi^*_p(x) g_\epsilon(x, 0) = \phi^*_p(0)/(\epsilon^+ - \epsilon_p);$$

$$\int dx g^*_\epsilon(x, 0) g_\epsilon(x, 0) = \frac{g^*_\epsilon(0, 0) - g_\epsilon(0, 0)}{\epsilon_2 - \epsilon_1 - i\eta};$$

$$\int d\epsilon g_{E-\epsilon}(x, 0)/(\epsilon^+ - \epsilon_p) = -2\pi i g_{E-\epsilon_p}(x, 0), \quad (16)$$
where the last equation represents the Kramers–Kronig relations.

To proceed, we need to specify $H_{sp}$. As the simplest possible example, we choose a simple $\delta$–function attractive potential,

$$H_{sp}(x) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - V \delta(x), \quad (17)$$

which has one bound state, $\phi_b = \sqrt{\kappa} e^{-\kappa|x|}$ with the inverse localization length $\kappa = mV/\hbar^2$, and with eigenenergy $-\epsilon_b = -\hbar^2 \kappa^2/(2m)$, and “band” scattering wave functions $\phi_p = (e^{ipx} + r_p e^{ip|x|})/\sqrt{L}$, with the reflection and transmission amplitudes

$$r_p = i\kappa/(p - i\kappa), \quad t_p = p/(p - i\kappa), \quad (18)$$

and with eigenenergy $\epsilon_p = \hbar^2 p^2/(2m)$. For this simple Hamiltonian one has \[14\]

$$g_\epsilon(x,x') = g_\epsilon(x',x) = -i\hbar\epsilon\epsilon_k|e^{-\kappa|x|} + r_k e^{ik_k(|x|+|x'|)}\rangle/(\hbar^2 k_\epsilon), \quad (19)$$

where the wave vector $k_\epsilon$ is defined by $k_\epsilon = \sqrt{2m\epsilon}/\hbar$, with $\Im k_\epsilon > 0$.

There are two physical situations which are of interest for the non–interacting wave function $\Psi_0^{pq}$. The first corresponds to two propagating electrons, impinging from the left, when both $p = p_1$ and $q = p_2$ represent “band” states. This yields the simple Eq. \[2\]. We devote the rest of this paper to the second, more interesting, choice for $\Psi_0^{pq}$, when one electron is propagating, with $p$ representing its wave vector, and the other is captured in the bound state “b”, i. e. $q = i\kappa$. Now the total energy is $E(p, b) = \epsilon_p - \epsilon_b \equiv \hbar^2 (p^2 - \kappa^2)/(2m) \geq -\epsilon_b$. In this case, the terms coming from the interaction are of the same order as the non–interacting ones, as now the amplitude for the two electrons to be together at $x = 0$ is of order $\sqrt{\kappa/L}$.

A long calculation, using Eqs. \[13\], \[14\], \[16\] and \[13\], now yields Eq. \[3\], and the effective transmission is given by

$$T(U, p) = |t_p|^2 - 2m\Re(F_E r_p t_p)/\hbar^2. \quad (20)$$

The second term here will have a “resonance” (yielding the large–$\kappa$ peak in Fig. 1) when the real part of the denominator of $F_E$ (cf. Eq. \[8\]) will vanish, i. e. when
\[ U_{\text{eff}}(E)^{-1} \equiv \Re(F_E^{-1}) = U^{-1} - \Re G_E^0(0, 0; 0, 0) \]  

(21)

vanishes. In some sense, \( U_{\text{eff}}(E) \) represents the renormalized interaction. The details of the transmission thus require explicit expressions for \( G_E^0(0, 0; 0, 0) \). Introducing an upper cutoff \( W = \hbar^2 \omega^2 / 2m \) on the “band” states, and using Eq. (14), we find (for real \( p \geq 0 \))

\[
\Re G_E^0(0, 0; 0, 0) = \frac{m}{\hbar^2} \left[ \frac{1}{4\pi} \ln y_c + \frac{\kappa^2}{\kappa^2 + p^2} \left( 1 - \frac{1}{\pi} \arctan \frac{W}{\epsilon_0} \right) \right. \\
+ \left. \frac{\kappa p}{\kappa^2 + p^2} \frac{1}{2\pi} \left( \ln \frac{\sqrt{W} + \sqrt{E + \epsilon_b}}{\sqrt{W} - \sqrt{E + \epsilon_b}} - \ln \left| \frac{y_c - y_1}{1 - y_c y_1} \right| \right) \right],
\]

(22)

with \( y_c = \left( 2\sqrt{W(W - E) + 2W - E} \right)^2 / E^2 \), \( y_1 = (p + \kappa)^2 / (p - \kappa)^2 \), and

\[
\Im G_E^0(0, 0; 0, 0) = -\frac{2m}{\hbar^2} \left[ \frac{p\kappa}{p^2 + \kappa^2} + \Theta(E)(\frac{p - \kappa}{2}) \frac{1}{p^2 + \kappa^2} \right],
\]

(23)

where \( \Theta(E) \) is the Heavyside function.

When \( p = 0 \), then \( G_E^0(0, 0; 0, 0) \) is real and the equation \( \Re G_E^0(0, 0; 0, 0) = 1/U \) (equivalent to the resonance \( U_{\text{eff}}(E)^{-1} = 0 \)) is identical to the equation for the transition from a doubly bound ground state to a ground state with one ‘free’ electron. \[12\] In our special case, \( \Re G_E^0(0, 0; 0, 0) \) starts at a negative value at \( \kappa = 0 \), changes to positive values around \( \kappa \approx 0.3 \), and approaches the asymptotic value 1/2 at large \( \kappa \). Thus, the above equation has a solution only for \( U > 2 \), when such a transition occurs. For small \( \kappa \), \( \Re G_E^0(0, 0; 0, 0) \) remains negative, \( U_{\text{eff}}(E) \) remains repulsive and there is no “resonance”; the transmission increases monotonically with \( U \), as shown in Fig. 3(a). For large \( \kappa \) (and \( p > 0 \)), \( U_{\text{eff}}(E) \) becomes negative, reflecting an attractive effective interaction! An explicit calculation now yields a peak in \( T(U, p) \) just before \( U_{\text{eff}}(E) \) changes sign, see Fig. 3(b). These results are understandable qualitatively: at small \( U \), the presence of the “bound” electron on the “dot” weakens the attractive potential \( V \), and thus causes an increase in the transmission. Indeed, a Hartree–Fock–like approximation, in which we calculate the average of the interaction term with the symmetrized wave function \( \Psi_0^{ph} \), yields \( V \to V - 2U\kappa \), and thus \( \kappa \to \kappa(1-2mU/\hbar^2) \). Using this renormalized value of \( \kappa \) in the bare transmission \( |t_p|^2 = p^2/(p^2 + \kappa^2) \), reproduces the result \[20\] in the small \( U \) limit. Thus, the interaction \( U \) compensates the (single–particle) attraction, and causes an increase in \( T(U, p) \). \[15\] When \( U_{\text{eff}}(E) \) changes sign and
becomes negative, the transmission has a pronounced peak. A similar dramatic behavior of $T(U, p)$ is manifested by its dependence on the depth of the single–particle bound state, $V$, or – equivalently – on $\kappa$, as shown in Fig. 1.

The above results indicate that the more interesting behavior of the transmission occurs when the single–particle attraction is high enough, $\kappa > \omega$ (that is, when the bound state energy $|\epsilon_b|$ is larger than the band width, $W$). In this situation, the total energy of the two electrons is negative [$p^2 < \omega^2 < \kappa^2$], and $\Im G^0_k$ is given only by the first term in Eq. (23). Then, the transmission takes an especially simple form

$$T(U, p) = |\tilde{t}_p|^2, \quad \tilde{t}_p = t_p \left(1 - F_p r_p\right) = t_p \left(\frac{1}{U_{\text{eff}}} + |r_p|^2\right) / \left(\frac{1}{U_{\text{eff}}} + i \frac{p\kappa}{p^2 + \kappa^2}\right).$$

(24)

Hence, when $1/U_{\text{eff}}$ approaches 0, $\tilde{t}_p \rightarrow -r_p$. At large values of $\kappa$ the reflection is close to unity. This explains the heights of the peaks in Figs. 2(b) and 4.

Returning to Eq. (22), it is interesting to note that the sign change in $\Re G^0_k$ originates from the last two terms, which vanish when $\kappa = 0$. In the absence of the bound state, $U_{\text{eff}}$ always remains negative. In the usual theory of superconductivity, the remaining first term in Eq. (22) renormalizes $U$ into a weaker repulsion, crucial for the superconducting state. All the interesting phenomena found here result from the additional effects of the bound state.

Finally, a comment about spins: starting with two general spins $\sigma_1$ and $\sigma_2$, one can always split the wave function into a combination of a singlet and a triplet. Without the interaction, the scattered electrons will have the same spins. Given the above results, the interaction will change the relative weights of the singlet and the triplet, and thus may cause a spin flip.

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REFERENCES

[1] M. A. Kastner, Comm. Cond. Mat. 17, 349 (1996); R. Ashoori, Nature 379, 413 (1996).

[2] L. P. Kouwenhoven et al., Phys. Rev. Lett. 65, 361 (1990).

[3] For a recent discussion, see, e.g., H. Ness and A. J. Fisher, cond-mat/9903320.

[4] D. Goldhaber-Gordon et al., Nature 391, 156 (1998).

[5] B. Su, V. J. Goldman, and J. E. Cunningham, Surf. Science 304, 566 (1994).

[6] T. K. Ng and P. A. Lee, Phys. Rev. Lett. 61, 1768 (1988); Y. Meir and N. Wingreen, Phys. Rev. Lett. 68, 2512 (1992).

[7] G. Grabert and M.H. Devoret (eds) Single Charge Tunneling, Coulomb Blockade Phenomena in Nanostructures, Nato ASI, Series B: Physics, Vol. 294 (Plenum, NY 1992).

[8] A. Georges and Y. Meir, Phys. Rev. Lett. 82, 3508 (1999).

[9] M. Wagner, U. Merkt, and A. V. Chaplik, Phys. Rev. B 45, 1950 (1992).

[10] B. E. Kane et al., cond-mat/9903371.

[11] B. E. Kane, Nature 393, 133 (1998).

[12] A. Aharony, O. Entin-Wohlman, and Y. Imry, Phys. Rev. B, 15 Feb. 2000 (cond-mat/9904182).

[13] P. W. Anderson, Phys. Rev. 124, 41 (1961).

[14] E. N. Economou, Green’s Functions in Quantum Physics (Springer-Verlag, Berlin 1979), Part II.

[15] The ‘screening’ found here is similar to the effective weakening of the disorder potential by interactions, reflected by the $h/e$ oscillations in mesoscopic rings [D. Weinmann et al., Phys. Rev. Lett. 75, 1598 (1995) and references there].
FIG. 1. The transmission $T(U,p)$ as function of $\kappa$ (in units of the cutoff $\omega$), for $U = 1, 2, 4$ (in units of $\hbar^2/(2m)$), solid line, and $T(0,p) = |t_p|^2$, dashed line. $p$ is in units of $\omega$. 
FIG. 2. The transmission $T(U,p)$ as function of the ‘bare’ interaction $U$ (in units of $\hbar^2/(2m)$). The solid line is $T(U,p)$, the dashed line shows $|t_p|^2$. (a) $\Re G_E^0 < 0$ ($\kappa = 0.2\omega$, $p = 0.04\omega$). (b) $\Re G_E^0 > 0$ ($\kappa = \omega$, $p = 0.1\omega$). The thick point signifies the change of sign of $U_{\text{eff}}$. 