Smearing of the Coulomb Blockade by Resonant Tunneling

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We study the Coulomb blockade in a grain coupled to a lead via a resonant impurity level. We show that the strong energy dependence of the transmission coefficient through the impurity level can have a dramatic effect on the quantization of the grain charge. In particular, if the resonance is sufficiently narrow, the Coulomb staircase shows very sharp steps even if the transmission through the impurity at the Fermi energy is perfect. This is in contrast to the naive expectation that perfect transmission should completely smear charging effects.

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The charge on an isolated metallic grain is quantized in units of the electron charge e. Even if the grain is weakly coupled to an electrode, so that electrons can occasionally hop from the electrode to the grain and back, the charge on the grain still remains to a large extent quantized. This phenomenon, known as Coulomb blockade, has in recent years been widely investigated, both theoretically and experimentally [1–3]. One quantity of interest is the average charge on the grain as a function of the voltage applied to a nearby gate. For a very weakly coupled grain this function shows very sharp steps, the so-called Coulomb staircase. As has been shown in recent experiments [4,5], the charge on such a grain can be directly measured using a single electron transistor that is capacitively coupled to the grain. The reason for the charge on the grain to be quantized is that it costs a finite energy $E_C = e^2/2C$ to charge the capacitance C formed by the grain and its environment. Charge quantization effects therefore become visible as soon as the temperature T is lowered below E_C. From now on we assume that the temperature is zero.

As the coupling of the grain to the lead is made stronger and stronger, the sharp steps of the Coulomb staircase are more and more smeared out. One usually assumes that all features of charge quantization completely disappear as soon as the coupling of the grain to the lead is via a perfectly transmissive channel [6–8]. However, this is the case only if the transmission probability from lead to grain is unity in an energy interval much broader than the charging energy E_C around the Fermi energy. We will show below that perfect transmission in a narrow energy interval is not sufficient to effectively smear out charging effects. We study a model where perfect transmission is achieved using a resonant impurity level connecting the grain to the lead. The transmission probability through such a resonant impurity level is strongly energy dependent and is characterized by the width Γ of the resonance. Embedding the level between sufficiently high tunneling barriers can give a small $\Gamma \ll E_C$. In this regime, one can achieve perfect transmission between the grain and the lead at the Fermi level and still have a nearly perfectly sharp Coulomb staircase. As the resonance is made wider, the sharp steps of the Coulomb staircase start to be smeared out and will eventually disappear at $\Gamma \gg E_C$.

The experimental setup we have in mind could, e.g., be a metallic grain, separated from a massive electrode by a thin insulating layer containing resonant impurity states near the Fermi level. Another possibility would be a double quantum dot system, where one of the dots is considerably smaller than the other (Fig. 1). The level spacing in the small dot then exceeds by far the charging energy of the larger one, so that the small dot can be occupied only by zero or one electron. The small dot plays then the role of the impurity. The advantage of this setup is that by tuning the gate voltages the barrier heights between the two dots and the lead can be adjusted. In addition, the effective energy of the impurity can be shifted by a gate which couples only to the small dot.

The model we consider is described by the following Hamiltonian:

$$H = H_0 + H_{li} + H_{ig} \, . \tag{1}$$

Here the Hamiltonian H_0 describes the lead, the impurity, and the grain,

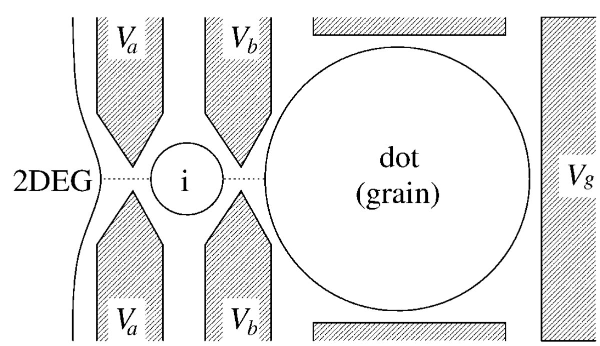

FIG. 1. A possible experimental setup using a GaAs heterostructure. The small quantum dot plays the role of the impurity level, and the larger dot represents the grain. The charge Q of the large dot is controlled by the gate voltage V_g. The voltages V_a and V_b control the heights of the barriers between the dots and the lead and thus the width of the resonance.

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$$H_0 = \sum_{k\sigma} \epsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \sum_\sigma \epsilon a^\dagger_\sigma a_\sigma + \sum_{p\sigma} \epsilon_p a^\dagger_{p\sigma} a_{p\sigma} + E_C(\hat{n} - N)^2, \tag{2}$$

and the coupling of the impurity to the other two electrodes is described by the tunneling Hamiltonians

$$H_{li} = \sum_{k\sigma} (t_k a^\dagger_{k\sigma} a_\sigma + \text{H.c.}), \tag{3}$$

$$H_{ig} = \sum_{p\sigma} (t_p a^\dagger_{p\sigma} a_\sigma + \text{H.c.}). \tag{4}$$

Here $a_{k\sigma}$, a_σ, and $a_{p\sigma}$ are the annihilation operators for electrons of spin σ in the lead, the impurity, and the grain, respectively. The operator $\hat{n} = \sum (a^\dagger_{p\sigma} a_{p\sigma} - \langle a^\dagger_{p\sigma} a_{p\sigma} \rangle_0)$ counts the number of electrons on the grain relative to its expectation value for the uncoupled system. The parameter N is proportional to the gate voltage V_g, namely, $N = C_g V_g / e$, where C_g is the capacitance between the grain and the gate electrode. In this model we neglected the interaction of electrons on the impurity site. We will later include a strong Coulomb repulsion on the impurity.

In the absence of tunneling, $H_{li} = H_{ig} = 0$, the charge $\langle Q \rangle$ on the grain is a multiple of the electron charge e, and thus is perfectly quantized. We will now investigate how the coupling via the impurity level affects the charge quantization on the grain. We assume that the coupling of the impurity to the grain is weak, so that it is sufficient to treat H_{ig} in perturbation theory. We can then take advantage of the fact that the system of an impurity coupled to a lead is noninteracting, and can therefore be easily solved exactly. Let $|0\rangle$ denote the ground state of the Hamiltonian (1) with $H_{ig} = 0$. The first order correction $|\delta\psi\rangle$ to $|0\rangle$ is

$$|\delta\psi\rangle = -i \int_{-\infty}^0 dt\, H_{ig}(t)\, |0\rangle, \tag{5}$$

where $H_{ig}(t)$ is the time evolution of the coupling taken in the interaction representation. The expectation value of the charge on the dot is then to second order in the coupling to the impurity

$$\begin{aligned}\langle Q \rangle = -e \sum_{p\sigma} |t_p|^2 \int_{-\infty}^0 dt_1 \int_{-\infty}^0 dt_2 \\ \times [\langle a_\sigma(t_2) a^\dagger_\sigma(t_1) \rangle \langle a^\dagger_{p\sigma}(t_2) a_{p\sigma}(t_1) \rangle \\ - \langle a^\dagger_\sigma(t_2) a_\sigma(t_1) \rangle \langle a_{p\sigma}(t_2) a^\dagger_{p\sigma}(t_1) \rangle],\end{aligned} \tag{6}$$

where the averages are taken over the ground state of the uncoupled system. The Green's functions of the isolated grain can be calculated easily:

$$\langle a^\dagger_{p\sigma}(t_2) a_{p\sigma}(t_1) \rangle = \theta(-\epsilon_p) e^{i(\epsilon_p - U_{-1})(t_2 - t_1)},$$
$$\langle a_{p\sigma}(t_2) a^\dagger_{p\sigma}(t_1) \rangle = \theta(\epsilon_p) e^{-i(\epsilon_p + U_1)(t_2 - t_1)}.$$

The Green's functions of the noninteracting impurity/lead system can be found by solving their equations of motion:

$$\langle a_\sigma(t_2) a^\dagger_\sigma(t_1) \rangle = \int_0^\infty \frac{d\omega}{\pi} \frac{\Gamma_l e^{-i\omega(t_2 - t_1)}}{(\omega - \epsilon)^2 + \Gamma_l^2},$$
$$\langle a^\dagger_\sigma(t_2) a_\sigma(t_1) \rangle = \int_0^\infty \frac{d\omega}{\pi} \frac{\Gamma_l e^{-i\omega(t_2 - t_1)}}{(\omega + \epsilon)^2 + \Gamma_l^2}.$$

Using these relations, the integrals in Eq. (6) can be evaluated and yield

$$\begin{aligned}\langle Q \rangle = 2e \frac{\Gamma_g}{\pi^2} \Bigg\{ \frac{U_1 - \epsilon}{\Gamma_l^2 + (U_1 - \epsilon)^2} \left[\frac{\pi}{2} - \arctan\left(\frac{\epsilon}{\Gamma_l}\right) + \frac{\Gamma_l}{U_1 - \epsilon} \ln \frac{\sqrt{\epsilon^2 + \Gamma_l^2}}{U_1} \right] \\ - \frac{U_{-1} + \epsilon}{\Gamma_l^2 + (U_{-1} + \epsilon)^2} \left[\frac{\pi}{2} + \arctan\left(\frac{\epsilon}{\Gamma_l}\right) + \frac{\Gamma_l}{U_{-1} + \epsilon} \ln \frac{\sqrt{\epsilon^2 + \Gamma_l^2}}{U_{-1}} \right] \Bigg\}.\end{aligned} \tag{7}$$

In this result we have five independent energy scales, namely, the couplings $\Gamma_g = \pi \sum_p |t_p|^2 \delta(\epsilon_p)$ and $\Gamma_l = \pi \sum_k |t_k|^2 \delta(\epsilon_k)$, the energy ϵ of the impurity, and, finally, the Coulomb energies $U_{-1} = E_C(1 + 2N)$ and $U_1 = E_C(1 - 2N)$, which have to be paid if an electron is removed from or added to the grain, respectively. We assume the energy spectrum in the lead as well as in the grain to be continuous. This implies that the grain is sufficiently large, so that the level spacing Δ is much smaller than all other relevant energy scales, $\Delta \ll \Gamma_{l,g}, U_{\pm 1}$. In this regime, the mesoscopic fluctuations of the coupling elements t_p will naturally average out in the expression for Γ_g.

Let us now discuss this result. Clearly, the charge smearing is linear in Γ_g, since we treated the coupling H_{ig} only to second order. The coupling H_{li} has been accounted for to all orders. Note that even if $\Gamma_l = 0$, i.e., the lead is decoupled from the rest of the system, the charge smearing does not vanish,

$$\langle Q \rangle = \mp 2e \frac{\Gamma_g}{\pi} \frac{1}{U_{\mp 1} \pm \epsilon}, \tag{8}$$

where the top and bottom signs correspond to positive and negative ϵ, respectively. This result can, of course, be easily obtained by performing a second-order perturbation theory with respect to H_{ig} in a system decoupled from the lead, $H_{li} = 0$. Clearly, the processes of multiple tunneling between the impurity and the grain result in corrections which are small in the parameter $\Gamma_g / U_{\mp 1}$. Therefore the lowest-order perturbation theory in H_{ig} employed in the derivation of Eqs. (8) and (7) is applicable away from the degeneracy points, i.e., at $\Gamma_g \ll U_{\pm 1}$.

As a next step, we investigate how the charge smearing is affected by the coupling to the lead, assuming now that both couplings Γ_l and Γ_g are finite. Let us first consider the case where the impurity level is far above the Fermi surface; i.e., we assume that $\epsilon \gg \Gamma_{l,g}, U_{\pm 1}$. Then Eq. (7) can be simplified to

$$\langle Q \rangle = -2e \frac{\Gamma_g}{\pi} \frac{1}{\epsilon} + 2e \frac{\Gamma_g \Gamma_l}{\pi^2 \epsilon^2} \ln \frac{U_{-1}}{U_1}. \tag{9}$$

The first term on the right-hand side coincides with Eq. (8) in the limit of large ϵ and is only due to the escape of electrons from the grain to the impurity. The second term is due to the transfer of electrons from the grain to the lead and is equivalent to the lowest-order result for charge smearing for a grain coupled to a lead via a tunneling barrier [9]. Comparing Eq. (9) with the result of Ref. [9], we find that charge smearing by tunneling via the impurity level is equivalent to that caused by tunneling through an effective barrier with the conductance $G = (e^2/\pi\hbar)4\Gamma_g\Gamma_l/\epsilon^2$. Naturally, this is exactly the conductance through the impurity in the limit of large ϵ.

As in the case of a simple tunneling barrier [9,10], the perturbative result diverges if one of the charging energies, U_1 or U_{-1}, approaches zero. The exact form of the charge smearing around the degeneracy points can be studied by mapping the system onto a 2-channel Kondo problem [10].

Equation (7) is particularly interesting in the regime where the impurity level is near resonance, $\epsilon \sim \Gamma$. Assuming that the gate voltage is sufficiently far from the degeneracy points, i.e., $\epsilon, \Gamma_{l,g} \ll U_{\pm 1}$, we can write Eq. (7) in the following compact form:

$$\langle Q \rangle = e \frac{\Gamma_g}{\pi} \left\{ \frac{n(\epsilon)}{U_1} - \frac{2 - n(\epsilon)}{U_{-1}} \right\}, \tag{10}$$

with the occupation of the impurity $n(\epsilon) = 1 - (2/\pi)\arctan(\epsilon/\Gamma_l)$. Since U_1 and U_{-1} are of the order of E_C, it is clear from this equation that for a narrow resonance the charge smearing is very small, of the order $\Gamma_g/E_C \ll 1$. This is the case even if the impurity level is on resonance, $\epsilon = 0$ and $\Gamma_l = \Gamma_g$, when the transmission at the Fermi energy is perfect, $T(E_F) = 1$. Physically, this result can be understood in the following way: in order to effectively smear out charging effects, the grain has to be perfectly coupled to the lead over an energy interval $\Delta E \gg E_C$ around the Fermi energy. However, in the case of resonant coupling, the transmission probability is strongly energy dependent. A resonant impurity level of width $\Gamma \ll E_C$ leads to perfect transmission only in the very narrow interval $\Delta E \sim \Gamma$. The transmission at all other energies essentially vanishes. To our knowledge, all previous work, that predicted charging effects to completely disappear as soon as there is at least one perfectly transmitting channel coupling the grain to a lead, assumed that the coupling is energy independent on the scale of E_C [7,8]. Our result clearly shows that a possible energy dependence in the coupling of the grain to the lead can have a dramatic effect on the shape of the Coulomb staircase.

In Fig. 2 the smearing of one step of the Coulomb staircase is shown for different values of the impurity energy ϵ. It is clearly visible that even at $\epsilon = 0$ the sharp Coulomb blockade step is only smeared out very little due to the narrow resonance, $\Gamma \ll E_C$. At $N = 0$ the slope of the Coulomb staircase with $\epsilon = 0$ is the same as the one found for a grain coupled through a tunneling barrier of effective conductance $G = (e^2/\hbar)2\Gamma_g/E_C$ to the lead. Therefore, away from the degeneracy points, a narrow resonant impurity level acts similarly to a poorly conducting tunneling barrier as far as charge smearing is concerned. However, if we approach a degeneracy point, e.g., $U_1 \ll (\Gamma_l + \Gamma_g)$, the smearing due to a resonant level is very different from the case of a tunneling barrier. At small U_1, the coupling of the grain to the lead, in fact, is strong, and thus the exact shape of the step of the staircase will differ considerably from the one found in [10]. Finding the exact shape of the step is a difficult task, which lies beyond the scope of this paper.

As the energy of the impurity is increased, the step of the staircase is pushed downwards, because the virtual processes of electron tunneling from the grain onto the impurity become more likely than processes where an electron from the partially occupied impurity tunnels onto the grain. However, in the limit of very large ϵ, hopping on the impurity becomes energetically more and more costly, so that the step moves back up again. This is illustrated in Fig. 3, where the charge on the grain is drawn for different fixed values of the gate voltage N as a function of the impurity energy ϵ. As the energy of the impurity crosses zero, the average charge makes an abrupt change from a positive to a negative value. The width of this jump is $\Delta\epsilon \sim \Gamma_l$. As can be seen from Eq. (10), measuring the average

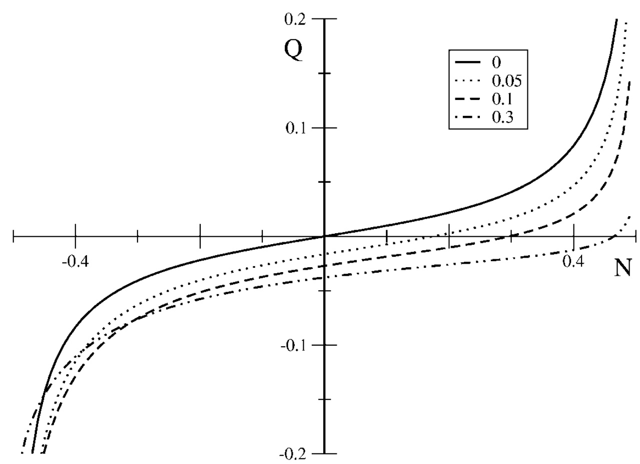

FIG. 2. The smearing of the Coulomb staircase, Eq. (7), for different values of ϵ/E_C. The coupling strengths have been chosen to be $\Gamma_l = \Gamma_g = 0.1E_C$. Drawn is the charge $\langle Q \rangle$ on the grain in units of the electron charge e as a function of the dimensionless gate voltage N. The divergences at the degeneracy points $N = \pm 0.5$ indicate the breakdown of the perturbative result at these points. Note the good quantization of the charge of the grain for $-0.4 < N < 0.4$, even if the impurity is on resonance (solid line).

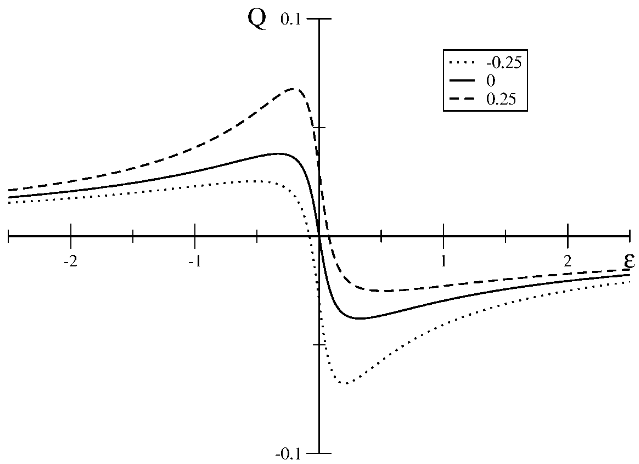

FIG. 3. The charge on the grain in units of e as a function of ϵ/E_C for different values of the gate voltage N. The couplings are $\Gamma_l = \Gamma_g = 0.1E_C$.

charge on the grain as a function of the impurity energy ϵ in this transition region is a direct measurement of the occupation $n(\epsilon)$.

Up to now we neglected the interaction of the electrons on the impurity. However, if in an experiment the impurity level is replaced by a second quantum dot in a heterostructure as suggested in the introduction, Fig. 1, it has to be much smaller than the large quantum dot, so that its charging energy U greatly exceeds the charging energy E_C of the dot. We will show now that a very similar result as Eq. (10) is also obtained if we include the strong Hubbard repulsion of the electrons on the impurity in our Hamiltonian. We add the following term to the Hamiltonian:

$$H_U = U\hat{n}_\uparrow \hat{n}_\downarrow, \tag{11}$$

with U being a very large energy, $U \gg E_C$, and $\hat{n}_\sigma = a_\sigma^\dagger a_\sigma$. The strong on-site Coulomb repulsion will now prohibit double occupation of the impurity level. To find the average charge on the grain, we can proceed with the so-modified Hamiltonian and rederive Eq. (6). Now the impurity Green's functions in Eq. (6) are nontrivial, because the Hamiltonian includes the on-site interaction (11). We consider a regime where the Coulomb energies U_1 and U_{-1} are much larger then ϵ. The Green's function of the impurity, $\langle a_\sigma^\dagger(t) a_\sigma(0)\rangle$, varies on a time scale $t \sim 1/\epsilon$, whereas the Green's functions $\langle a_{p\sigma}^\dagger(t) a_{p\sigma}(0)\rangle$ vary on the much shorter time scale $t \sim 1/U_{-1}$. We can therefore assume that the Green's function of the impurity is roughly constant in the relevant range of integration over t_1 and t_2, and is given by $n(\epsilon) = \sum_\sigma \langle a_\sigma^\dagger a_\sigma\rangle$. The integrals in Eq. (6) can then be carried out, and we arrive at the same result as Eq. (10), except that in the presence of interactions on the impurity $n(\epsilon)$ is the occupation of the impurity in the Anderson model $H_0 + H_{li} + H_U$. As can be seen from Eq. (10) and Fig. 3, the measurement of the charge on the grain can be used to determine the occupation $n(\epsilon)$ of the Anderson impurity.

In this paper we have studied the influence on the Coulomb blockade of a strong energy dependence of the coupling of a grain to its environment. The example we investigated was a grain, which was coupled to a lead via a resonant impurity level. Charge smearing by this coupling has two origins: first, the sole presence of a nearby impurity can already smear the charge on the grain even without any coupling to the lead. The second reason for charge smearing is due to transfer of electrons from the grain over the impurity to the lead. We showed that a narrow resonance, $\Gamma \ll E_C$, is not sufficient to effectively smear out charging effects. It is worth noting that our result is not related to the phenomenon of mesoscopic charge quantization [11], which results in small Coulomb blockade oscillations in a perfectly coupled small quantum dot. Unlike Ref. [11], our Coulomb blockade oscillations can be large, and they do not disappear in the limit of vanishing level spacing in the dot. We also showed that the charge on the grain can be used to measure the occupation of the impurity; see Eq. (10). The easiest way to experimentally verify our prediction is probably to use a double dot system in a semiconductor heterostructure, where one of the dots plays the role of the impurity, Fig. 1.

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[1] D. V. Averin and K. K. Likharev, in *Mesoscopic Phenomena in Solids,* edited by B. Altshuler, P. A. Lee, and R. A. Webb (Elsevier, Amsterdam, 1991).
[2] *Single Charge Tunneling,* edited by H. Grabert and M. H. Devoret (Plenum Press, New York, 1992).
[3] L. P. Kouwenhoven, C. M. Marcus, P. L. McEuen, S. Tarucha, R. M. Westervelt, and N. S. Wingreen, in *Mesoscopic Electron Transport,* edited by L. L. Sohn, L. P. Kouwenhoven, and G. Schön (Kluwer, Dordrecht, 1997).
[4] P. Lafarge, P. Joyez, D. Esteve, C. Urbina, and M. H. Devoret, Nature (London) **365**, 422 (1993).
[5] D. Berman, N. B. Zhitenev, R. C. Ashoori, and M. Shayegan, Phys. Rev. Lett. **82**, 161 (1999).
[6] N. C. van der Vaart, A. T. Johnson, L. P. Kouwenhoven, D. J. Maas, W. de Jong, M. P. de Ruyter van Steveninck, A. van der Enden, C. J. P. M. Harmans, and C. T. Foxon, Physica (Amsterdam) **189B**, 99 (1993).
[7] K. A. Matveev, Phys. Rev. B **51**, 1743 (1995).
[8] Yu. V. Nazarov, Phys. Rev. Lett. **82**, 1245 (1999).
[9] L. I. Glazman and K. A. Matveev, Sov. Phys. JETP **71**, 1031 (1990).
[10] K. A. Matveev, Sov. Phys. JETP **72**, 892 (1991).
[11] I. L. Aleiner and L. I. Glazman, Phys. Rev. B **57**, 9608 (1998).