In-phase resonances and the Coulomb blockade effect

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Using the simple arguments we argue that the large charging energy leads naturally to the in-phase charge-transfer resonances through the quantum dot with one-dimensional leads.

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The famous experimental work by Yacoby et al [1], (where the magnitude t_0 and phase θ of the transmission coefficient $t = t_0 e^{i\theta}$ through the quantum dot embedded in an Aharonov-Bohm ring in the Coulomb blockade regime were measured) initiates a great activity [2]-[21] directed to explain the unusual observed behaviour of the phase θ of the transmission coefficient that can not be understood within the simple single-electron picture. It was observed, firstly, that the phase of Aharonov-Bohm oscillations of ring's conductance $G(\Phi)$ (where Φ being a magnetic flux through the ring's opening) changes abruptly when the transmission coefficient t of a quantum dot passes through the Coulomb blockade peak maximum and, secondly, that the Aharonov-Bohm oscillations at consecutive conductance peaks are in phase.

As it was established [2, 5] the first feature is a direct consequence of a symmetry of a two-terminal conductance $G(\Phi) = G(-\Phi)$. This implies that the phase shifts δ_n in a Fourier representation of a conductance $G(\Phi) = G_0 + \sum_{n=1}^{\infty} G_n \cos(2\pi n\Phi/\Phi_0 + \delta_n)$ (here $\Phi_0 = h/e$ being the flux quantum) may be zero or π only. Usually the first harmonic dominates $G_1 > G_n,\ n > 1$, therefore δ_1 is an experimentally observable phase shift [1]. Because of interference the conductance of a ring depends on the phase accumulated by an electron traveling along the arms of a ring. Thus, δ_1 depends on the phase θ of the transmission coefficient t through the quantum dot. Near the transition resonance the phase θ changes by π that leads to an abrupt change of δ_1 from 0 to π (or vice versa). More precisely, the mechanism of such a change is as follows [3, 5, 7, 13]. Near the maximum of t the first harmonic of ring's conductance vanishes and the dependence $G(\Phi)$ becomes a $\Phi_0/2$-periodic in a magnetic flux (the second harmonic dominates). At further change of t the dependence $G(\Phi)$ becomes Φ_0-periodic again with δ_1 being changed.

The second feature, confirmed by further experiments [22, 23], is more difficult to explain. The single-particle picture naturally leads to out of phase resonances [1]. This is due to the fact that the phase of the transmission coefficient changes by π when we go consecutively from one resonance to another one. To illustrate this we will follow to Ref.[5] and consider the quantum dot containing noninteracting electrons within a one-dimensional double-barrier resonant tunneling model. The transmission coefficient t through the two identical delta function potential barriers of strength $U_0 \gg \epsilon_F$ (where ϵ_F is the Fermi energy) separated by the distance L may be represented as a sum of the Breit-Wigner [24] resonances

$$t = e^{-ikL} \sum_n \frac{-i\Gamma_n/2}{E_k - E_n + i\Gamma_n/2}, \tag{1}$$

where $E_k = \hbar^2 k^2/(2m)$ is an electron energy; E_n and $\Gamma_n > 0$ are the energy and broadening of the resonance n. In the limit of a small coupling between the quantum dot and the leads $\Gamma_n \ll \Delta_F$ (where Δ_F is the level spacing in the dot near the Fermi energy) the resonant energies E_n with a good accuracy are the energies of single-electron levels in an isolated dot $E_n = \hbar k_n^2/(2m)$; $k_n = \pi n/L$, $n = 1, 2, \ldots$. Near a resonance ($k \simeq k_n$) the exponential term in Eq.(1) gives $t \sim e^{-i\pi n}$. Thus, at successive resonances ($\Delta n = 1$) the change of a transmission coefficient phase is π. Note, that the four-terminal measurements [23] (where the magnitude t_0 and the phase θ of the transmission coefficient through the quantum dot are measured directly) confirm that the behaviour of θ near a resonance peak is well described by a single electron model. So, near a resonance we can use the representation Eq.(1), but to explain the in-phase feature of resonances we must suppose that the phase θ changes by π (up to 2π) between resonances that is not described by Eq.(1).

Another consideration [2], based on the Friedel sum rule [25], leads also to out of phase resonances for noninteracting electrons. Following the Landauer-Büttiker approach [26, 27] let us consider the quantum dot connected to two one-dimensional leads as a phase coherent scatterer. The (spinless) Friedel sum rule relates the change of an electron phase (in our notation θ) due to scattering to the charge of a scatterer (of a quantum dot) $Q_D = -eN_e$ (here $-e$ is an electron charge, N_e is the number of electrons in a quantum dot)

$$\theta = \pi Q_D/e. \tag{2}$$

After each resonance one electron is added to the quantum dot $\Delta N_e = 1$. Therefor the transmission coefficient phase θ at successive resonances changes by π: $\Delta\theta = \pi\Delta N_e = \pi$.

To overcome this discrepancy with experiments [1, 22, 23] a number of efforts have been made. Ref.[2] suggests an accumulation of a fractional charge αe (when the voltage V_g of a gate capacitively coupled to a quantum dot varies) in the ring between the two resonances. Since the phase of the dependnece $G(\Phi)$ may be zero or

π only, this may explain the parity conservation at limited number of peaks. Some other considered physical effects are: multiple tunneling through exactly the same state of a dot [3, 8, 12]; the strong Coulomb interaction [3, 4]; the finite temperatures [9]; the intrinsic properties of a ring-like structure [14]; the interplay of interelectron interactions and the coupling to leads that may lead to the suppression of some resonance peaks [19]. A number of works [6, 15–18, 21] exploits the 2D (in contrast with the purely 1D models) nature of a quantum dot. In these models the phase change π between resonances does not connect with an additional charge but arises due to the transmission zeros which are produced by the bound states. As it was shown in Refs.[18, 21], in the presence of transmission zeros the Friedel sum rule Eq.(2) must be generalized to take into account the fact that near a transmission zero the phase θ of the transmission coefficient changes by π without any change in an electron charge of a quantum dot. However, because of the absence of any known regularity in arising of transmission zeros, this mechanism may explain the presence of a small number of off-phase resonances [23] rather than regularly arising in-phase resonances.

In the present paper we demonstrate that the intrinsic feature of the Coulomb blockade effect leads naturally to in-phase resonances regardless of interelectron interactions within a quantum dot, an electron spin, and the dimension (either 1D or 2D) of a quantum dot.

As it well known the Coulomb blockade effect [28] consists in as follows. At low temperatures the charging energy connected with a small capacitance C of a mesoscopic sample (of a quantum dot) affects considerably the electron transport through the quantum dot coupled via tunnel junctions to an environment. Electron tunneling through the potential barrier changes the charge of a quantum dot by $1e$ that changes the energy E of the system by $\Delta E \sim E_c = e^2/(2C)$. Note that for the mesoscopic system the typical capacitance is $C \leq 10^{-15}F$, that corresponds to $E_c \geq 1K$.

At low temperatures

$$T \ll E_c, \tag{3}$$

in the common case the charge transfer is suppressed (the Coulomb blockade effect) [29, 30] and the conductance of a quantum dot is very small. However, at some values of a potential V_g of the gate capacitively coupled to a quantum dot the electrostatic energy $\mathcal{E}$

$$\mathcal{E}(N_e) = E_c(Q_p/e - N_e)^2 \tag{4}$$

(where $Q_p = C_g V_g$ is the polarization charge of a quantum dot induced by the gate with a capacitance C_g) may be degenerate in N_e

$$\mathcal{E}(N_e) = \mathcal{E}(N_e + 1). \tag{5}$$

In this case the Coulomb blockade is lifted and the conductance of a quantum dot peaks.

Such degeneracy occurs at half-integer values of Q_p [31, 32] when the charge $Q_D = Q_p - eN_e$ of a quantum dot equals to

$$Q_D = e/2. \tag{6}$$

When we pass over the Coulomb blockade resonance the number of electrons in the dot changes by 1 and the charge of a dot Q_D (with accounting of a polarization charge Q_p) changes from $e/2$ before resonance to $-e/2$ after resonance. To obtain the next resonance (see Eq.(6)) we must vary the gate voltage V_g to change Q_p (and consequently Q_D) by $1e$ exactly (from $-e/2$ to $e/2$). Therefore, between Coulomb blockade resonances the charge of a dot changes by $1e$ that is due to a polarization charge induced by the gate and does not connect with the charge transfer between the dot and the leads. So, we see that the condition of the Coulomb blockade resonance Eq.(6) requires the same charge of a quantum dot near each peak of a conductance. Applying the Friedel sum rule Eq.(2) we conclude that the transmission coefficient phase θ is *exactly* the same near the Coulomb blockade resonances and all the resonances are in phase. Note, that the effect of a partial change of the charge of a quantum dot between resonances was considered by Yeyati and Büttiker [2] but in the present paper we emphasize that the condition of a degeneracy of a charging energy (needed to obtain the Coulomb blockade peak) requires the *exactly* $1e$ change of the charge of a quantum dot between resonances.

This conclusion is also valid if we include interelectron interactions. Note, that if we take into account a charging energy Eq.(4) (which is due to a long-range Coulomb interaction) we, in fact, consider (even initially free) electrons as interacting particles. In addition, now we consider the effect of (short-range) electron-electron interactions within a quantum dot. The Hamiltonian $\hat{H}$ of a system (interacting electrons in the quantum dot and noninteracting electrons in leads) is

$$\hat{H} = \hat{H}_0 + E_c(Q_p/e - \hat{N}_e), \tag{7}$$

where $\hat{H}_0$ is the Hamiltonian of a system without a charging energy (the second term in RHS of Eq.(7)); $\hat{N}_e = \sum_p c_p^\dagger c_p$ is the operator of the number of electrons in the dot. Note, that we describe a charging energy within a geometrical capacitance approach which is widely used when the Coulomb blockade effect is considered. In experiment Ref.[1] the temperature T was less than the level spacing $\Delta_F \sim \epsilon_F/N_e$ ($N_e \gg 1$) in the dot. Therefore analyzing dot's conductance we may consider the tunneling processes in (and out of) the ground state of a quantum dot only. At weak coupling between the quantum dot and the leads the number N_e of electrons in the quantum dot is well quantized (see e.g., [33]) (except narrow vicinities of a charge transfer resonance where the number of electrons in the quantum dot fluctuates between N_e and $N_e + 1$). Thus, in the limit of a weak coupling between the quantum dot and the leads (that is the case in the experiment Ref.[1]) the charge transfer resonance occurs when the ground state energy E_0 of a system of interacting electrons degenerates in the number of electrons in the dot: $E_0(N_e) = E_0(N_e+1)$ (in the case of noninteracting electrons this condition means that the Fermi energy ϵ_F of electrons in leads coincides with a one of the single-electron levels in the quantum dot). So, we need to know the ground state energy E_0 of the Hamiltonian Eq.(7) as a function of N_e. Let us estimate the change in E_0 due to the change of the number of electrons in the dot. There are two origins of such a change. The first origin due to the dependence of the energy of a system of interacting electrons in the quantum dot on the number of particles. This change is of the order of $\delta E_0^{(1)} \sim \Delta_F \sim \epsilon_F/N_e$. The second origin is due to a charging energy $\delta E_0^{(2)} \sim E_c$. To compare these quantities we use the data of an experiment Ref.[1]: $E_c \approx 500\mu eV$; $\Delta_F \approx 40\mu eV$; $T \approx 9\mu eV$; $\Gamma \approx 0.2\mu eV$. So, in addition to Eq.(3) further we will assume

$$E_c \gg \Delta_F \gg \Gamma, \tag{8}$$

(Γ is the level broadening due to tunneling in and out of the quantum dot) In such a case the charging energy is a dominant energy scale which determine the dependence of the ground state energy on the number of electrons in the quantum dot $\delta E_0^{(2)} \gg \delta E_0^{(1)}$. Thus, in the Coulomb blockade regime Eqs.(3),(8) the resonance condition (even for interacting electrons) is the condition of a degeneracy of a charging energy $\mathcal{E}$ Eq.(5) which implies Eq.(6). So, using the Friedel sum rule (which remains valid in the presence of electron-electron interactions as it was shown by Langer and Ambegaokar [34]) we conclude that all the Coulomb blockade resonances must be in phase.

So far we ignore an electron spin. Now we show that the inclusion of an electron spin does not change an in-phase feature of the Coulomb blockade resonances. For spinfull case the Friedel sum rule Eq.(2) reads $\theta = \pi Q_D/(2e)$. In the case of noninteracting electrons the energy levels in the quantum dot are twofold (spin-) degenerate and at resonance two electrons enter the quantum dot. So, for noninteracting spinfull electrons the consecutive peaks are out of phase (like for spinless electrons). The inclusion of a charging energy $\mathcal{E}$ makes electrons interacting and removes the spin degeneracy of energy levels in the quantum dot.

As it well known at $T = 0$ the Kondo effect develops if spinfull interacting electrons tunnel through the quantum dot [35]. However, in the limit of a weak coupling the Kondo temperature is very small [36] and at actual experimental temperatures [1] the system is out of the Kondo regime. In the absence of Kondo-like correlations the main effect of electron-electron interaction (which is mainly due to a charging energy $\mathcal{E}$ in the Coulomb blockade regime Eq.(8)) is the remove of a spin degeneracy and the definition of the charge transfer resonance condition Eq.(5) which leads to Eq.(6). Thus, because of the same charge of a quantum dot Eq.(6) near a resonance the Coulomb blockade peaks are in phase as well as in the spinless case.

Now we examine more accurately the behaviour of the phase of the transmission coefficient near two consecutive resonances arising from the level of a quantum dot which is spin-degenerate in the absence of a charging energy. To this end we consider a resonant transport through a single twofold (spin-) degenerate level with on-site Coulomb repulsion $U \sim E_c$ [35] (the one-impurity Anderson model). The model Hamiltonian is

$$\hat{H} = \hat{H}_0 + \epsilon_0 \sum_{\sigma=\uparrow,\downarrow} \hat{n}_{0\sigma} + U\hat{n}_{0\uparrow}\hat{n}_{0\downarrow}. \tag{9}$$

Here Hamiltonian $\hat{H}_0$ describes the free electrons in one-dimensional (right and left) leads and tunneling between the leads and the dot; ϵ_0 is the energy of the level in the dot; $\hat{n}_{0\sigma} = c^\dagger_{0\sigma}c_{0\sigma}$ is the electron number operator. In the case of a symmetric coupling to the leads the transmission coefficient is [35, 37]

$$t(\epsilon) = -iG^r(\epsilon)\Gamma/2, \tag{10}$$

where $\Gamma = 2\pi N(\epsilon)t_t^2$ is the broadening (the tunneling rate); $N(\epsilon)$ is the density of states for electrons in leads at the energy ϵ; t_t is the tunneling matrix element. Neglecting Kondo-like correlations we can use an approximate retarded Green's function G^r of the Breit-Wigner type [37]

$$G^r(\epsilon) = \frac{1-\langle n\rangle/2}{\epsilon-\epsilon_0+i\Gamma/2} + \frac{\langle n\rangle/2}{\epsilon-\epsilon_0-U+i\Gamma/2}. \tag{11}$$

The self-consistent value of the occupation on the dot is $\langle n\rangle = (1+2P_1)/(1+P_1-P_2)$, where $P_i = \pi^{-1}\arctan(2\Gamma^{-1}\delta\epsilon_i)$, $i = 1,2$, $\delta\epsilon_1 = \epsilon-\epsilon_0$, $\delta\epsilon_2 = \epsilon-\epsilon_0-U$ [37]. Using these expressions we can easy calculate the phase θ of the transmission coefficient near the two resonances: $\theta(\epsilon) = \theta_1(\epsilon)$ at $\epsilon \approx \epsilon_0$ and $\theta(\epsilon) = \theta_2(\epsilon)$ at $\epsilon \approx \epsilon_0 + U$, where

$$\tan(\theta_i) = \frac{2}{\Gamma}\left(\delta\epsilon_i - A_i\frac{\delta\epsilon_i^2+\Gamma^2/4}{U}\right). \tag{12}$$

Here $A_1 = \left(\frac{2}{\langle n\rangle}-1\right)^{-1}$; $A_2 = \left(1-\frac{2}{\langle n\rangle}\right)$. Easy to see that in the limit of a large charging energy ($U \gg \Gamma$) the behaviour of the phase θ is the same near the two resonances.

Below we discuss briefly the case of a quasi-1D quantum dot. All arguments leading to Eqs.(5),(6) remain valid, but the Friedel sum rule Eq.(2) must be modified because of a possible appearance of transmission zeros [18, 21]. The transmission zero leads to an additional change π of the phase θ of the transmission coefficient and breaks off the series of in-phase Coulomb blockade resonances.

In summary, we demonstrated that the conventional picture of the Coulomb blockade effect leads naturally to the in-phase resonances of the conductance of a quantum dot with one-dimensional leads that is in agreement with experimental observations [1, 22, 23].

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