An Approximate Sign Sum Rule for the Transmission Amplitude through a Quantum Dot

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We study the phase of the transmission amplitude through a disordered quantum dot in the Coulomb blockade regime. We calculate the phase dependence on gate voltage for a disorder configuration. We show that over a "period," consisting of a resonance and a transmission valley, the total phase change is $0 \pmod{2\pi}$. Deviations from this sum rule are small in the parameter (level spacing and/or charging energy). The disorder-averaged phase-phase correlation function is found showing interaction-induced correlations between phases at different gate voltages.

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The physics of quantum dots (QD) has been the subject of intense theoretical and experimental studies in recent years. Most of those studies focused on the role of the Coulomb blockade (CB) in defining quantum transport through such systems. Two novel interference experiments [1,2] studied coherence and transmission phase rather than transmission probability—evolution in QD as a function of the Aharonov-Bohm flux Φ and the gate voltage V_g . The flux controls the relative phase through the two arms of the interferometer while the gate voltage drives the dot in and out of resonance, controlling the mean number of electrons on the dot. The first experiment [1], employing a two terminal setup, restricted the relative phase of the interferometer (at $\Phi = 0$) to be either 0 or π . In the second experiment the setup was similar to a two-slit interferometer and the (relative) phase of the transmission amplitude through a QD in the CB regime could be measured.

Several interesting aspects of the experimental data have been subsequently discussed in the literature; see, e.g., [3]. The most intriguing result though, discussed below, has remained unaccounted for. It has to do with the evolution of the transmission phase through the dot, α , as V_g is varied, scanning resonances and the "transmission valleys" between them. Hereafter we attach an index N to a valley, corresponding to the number of electrons on the dot over that range of V_g . The resonance separating the valleys N-1 and N will be denoted by (N-1,N). We shall parametrize V_g in the valley by x: for the valley N the parameter $x \to 0$ corresponds to the right of resonance (N-1,N), i.e., the point where the energies of the dot with N-1 electrons and N electrons are practically degenerate; $x \rightarrow 1$ corresponds to the left of resonance (N, N + 1). A complete description of V_g is given by the two variables (N, x). The remarkable result of the experiment is that as V_g is varied the change in the transmission phase $\Delta \alpha$ between two consecutive valleys turns out to be $0 \pmod{2\pi}$. This is in distinct contrast to the behavior of noninteracting electrons in one-dimensional symmetric dots, where $\Delta \alpha = \pi$, or two-dimensional dots where, depending on the details of the geometry and disorder, $\Delta \alpha$ forms a sequence of 0 and π .

There is a large number of works addressing the remarkable transmission phase correlations observed in the experiments. While we shall not present here a critical review of all those attempts, it is worthwhile noting that each of those works is subject to at least one of the following critiques: (i) An implicit assumption is made concerning the matrix elements coupling the dot to the leads. (ii) A rather particular geometry or potential is considered. (iii) Restrictive ranges of parameters are assumed.

Motivated by the experiment we present here a mechanism which accounts for phase correlations for different values of V_g . Our theory contains two desirable features which were missing from previous works: (i) Our mechanism is generic and does not invoke the peculiarities listed above. (ii) We identify a large dimensionless parameter in the light of which our theory is formulated. Our analysis pertains to individual, disorder specific systems. In addition we also calculate the disorder-averaged phase-phase correlation function which depends on the gate voltage and observe interaction-induced correlations.

We argue below that as V_g is varied there are three distinct mechanisms for t to acquire a phase change of π : there is an increase by π as the gate voltage is swept through a resonance; between resonances we may encounter a near-resonance phase lapse (NRPL) and a valley phase lapse (VPL), each involving a phase change of π .

Our sum rule states that the *number* of π changes between consecutive valleys due to all these mechanisms is even, resulting in $\Delta \alpha = 0 \pmod{2\pi}$. The frequency of deviations from this sum rule is small in Δ/U where Δ is the mean single particle level spacing and U is the charging energy of the dot.

We consider an Aharonov-Bohm (AB) interferometer where a QD is embedded in one arm. The arm containing the QD can be modeled by the Hamiltonian

$$H = H^{L} + H^{R} + H^{QD} + H^{T}, (1)$$

$$H^{L(R)} = \sum_{k} \varepsilon_k a_k^{L(R)\dagger} a_k^{L(R)}, \qquad (2)$$

$$H^{T} = \sum_{k,j} V_{j,k}^{L} c_{j}^{\dagger} a_{k}^{L} + \text{H.c.} + L \leftrightarrow R, \qquad (3)$$

$$H^{\rm QD} = \sum_{j} (\epsilon_j - eV_g) c_j^{\dagger} c_j + \frac{U}{2} \hat{N}(\hat{N} - 1). \tag{4}$$

 $H^{L,R}$ describes the regions to the left and right of the QD, H^T represents the tunneling of electrons in and out of the QD, and $H^{\rm QD}$ describes the states of the isolated QD with the constant interaction term.

The total transmission probability through the AB interferometer, T(E), is the modulus squared of the sum of the transmission amplitudes through the two arms, t(E) and t_0 [the latter refers to the free arm and is assumed to be constant, $|t_0| \gg |t(E)|$]. Since the entire interferometer is coupled to external reservoirs, T(E) needs to be convoluted with the Fermi function f,

$$T = \int dE \left(-\frac{\partial f}{\partial E} \right) |t(E) + t_0|^2$$

$$\approx |t_0|^2 + 2\operatorname{Re} t_0^* \int dE \left(-\frac{\partial f}{\partial E} \right) t(E). \tag{5}$$

We first propose a qualitative picture which motivates and expounds the phase correlations. Figure 1 depicts (schematically) virtual processes (second order in the V's) which, at zero temperature, contribute to the transmission amplitude, say, from the left lead (L) to the right lead (R). An off-resonance (valley) setup is shown. There are electron-like processes, employing vacant levels (e.g., ϵ_i) as intermediate states. The contribution of such a process to t(E) is (neglecting corrections due to level broadening) $\sim V_j^L V_j^{R*} / [E - (\epsilon_j - eV_g + UN) + i\Gamma]$ where $V_j =$ $V_{i,k(E)}\sqrt{2\pi\rho(E)}$ with N electrons on the QD. Here, ρ is the density of states in the left or right lead. We focus on a disordered QD where $\{\epsilon_i\}$ and $\{V_i\}$ are fluctuating and are described to a good approximation by random matrix theory. The numerator thus has a random sign (in the absence of a magnetic field it can be chosen real).

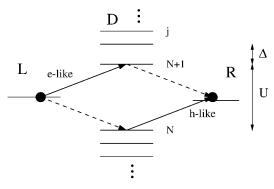


FIG. 1. Level scheme out of resonance, depicting electronlike and holelike processes.

The contributions of the electronlike processes to t(E) arise from a large number of random terms (of which $\sim U/\Delta$ contribute significantly). We denote the sum over the contributions with $j \geq N+2$ ($j \leq N-1$) the "electron team" ("hole team") [4]. The contribution of the j=N+1 level (j=N) will be referred to as the "electron team captain" ("hole team captain").

The following observations are now due: (a) The signs of the four contributions (the "teams" and the "captains") are random, however, the teams in the Nth valley and in the (N+1)th valley differ very little from each other (essentially by the contribution of one level). Thus, up to events which are rare by the parameter Δ/U , the signs of the e teams (h teams) in two consecutive valleys are the same. (b) As eV_g is increased in the valley the magnitude of the e team (h team) increases (decreases). Furthermore, as the resonance is approached, the relative importance of the team diminishes and eventually near the resonance it is a single level—the team captain—which governs the transmission.

A phase lapse occurs when the signs of the e team and the h team differ (VPL) or when a team does not agree in sign with its captain (NRPL). Figure 2 depicts the evolution of the e contributions and the h contributions to Ret over a range of V_g . In Fig. 2 we display the signs of the four contributions to be e team = +, e team captain = +, h team = -, h team captain = -. A VPL occurs and the total number of phase gains by π over a period is 2, rendering $\Delta \alpha = 0 \pmod{2\pi}$. Evidently one needs to examine each of the 16 possible sign assignments, each yielding a different pattern of t as a function of V_g . But remarkably enough we find that over a period as defined above π (at resonance) + π (number of NRPL) + π (number of VPL) = even.

Next we put the above picture in a more quantitative framework. The transmission amplitude through the interacting system is linked to the retarded Green's function G_{ij} of the QD coupled to the leads by $t(E) = \sum_{ij} V_i^L V_i^{R*} G_{ij}$. As we are interested in the elastic

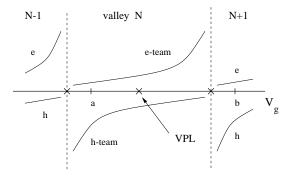


FIG. 2. The evolution of the e contribution and the h contribution to Ret as a function of V_g (schematic); \times denotes a phase change of π . See text for the choice of the signs for the "teams" and "captains" contributions. The total phase change over a period [say from $V_g(a)$ to $V_g(b)$] is 0 (mod π).

cotunneling contributions [5] rendering G_{ij} diagonal (tunneling in and out of the same dot state), G_{ij} can approximately be determined by iterating the equation of motion. Specifically we use an extension of Ref. [6] to many levels in the dot,

$$t(E) = \sum_{j} V_{j}^{L} V_{j}^{R*} \sum_{N=0}^{\infty} P_{N} \left(\frac{\langle n_{j} \rangle_{N}}{E - (\epsilon_{j} - \epsilon_{N} - xU) + i\Gamma_{j}} \right) + \left(\frac{1 - \langle n_{j} \rangle_{N}}{E - [\epsilon_{j} - \epsilon_{N} + (1 - x)U] + i\Gamma_{j}} \right).$$
(6)

$$\langle \cdots \rangle_N = \operatorname{tr}_N \exp{-\beta H^{\mathrm{QD}}} \dots / \operatorname{tr}_N \exp{-\beta H^{\mathrm{QD}}}$$

denotes

thermal average with N electrons. The probability to find N electrons on the QD is given by $P_N = \langle \hat{N} \rangle_N / \sum_M \langle \hat{N} \rangle_M$. Deep in the valley N we have $P_M \simeq \delta_{M,N}$. The two terms of (6) describe the h-like and the e-like contributions, respectively [7].

For the sake of simplicity the statistics we first introduce is a toy model (to be revoked later), with the assumptions that (i) the level spacing is constant $\epsilon_j = j\Delta$ mimicking the level repulsion and (ii) $V_j^L V_j^{R*} = V \eta_j$ where η_j is a random variable which can take the values +1 and -1 with equal probability. This models the fluctuations in the wave function due to disorder. The relevant physics is already contained in the toy model as a comparison with random-matrix-generated energies and couplings reveals. Let us first consider the noninteracting case. The transmission amplitude then becomes

$$t(E) = V \sum_{j} \frac{\eta_{j}}{E - (\epsilon_{j} - eV_{g}) + i\Gamma}, \qquad (7)$$

where the system can be tuned in or out of resonance by the gate voltage eV_g . At the resonance α increases by π . The signs of η_j govern the phase evolution between the resonances. If $\eta_1 \cdot \eta_2 > 0$ there is a decrease by π (phase lapse) between the resonances 1 and 2; for $\eta_1 \eta_2 < 0$ this phase lapse is absent. Note that in a one-dimensional symmetric potential η_j alternates in sign implying no phase lapse. For a disordered noninteracting QD the phase lapses occur at random [10]. Here we show that interaction changes this picture considerably.

We note that near the resonances (N-1,N) the main contribution to t in (6) comes from the electron contributions of the N-1 valley and the hole contribution of the N valley. The other contributions are smaller by a factor of U/Δ . At the resonance (N-1,N) the level ϵ_N is resonating which is the e-team captain in the N-1 valley and the h-team captain in the N valley. When we single out the state ϵ_N in the electron and hole states we see that the vicinity of (N-1,N) is equivalent to the single particle resonance of level ϵ_N , $\eta_N/[E-(\epsilon_N-eV_g)+i\Gamma]$ and background term A_{N-1} and B_N corresponding to the e team (N-1) valley) and the h team (N) valley). These background terms for different valleys are

strongly correlated, e.g., the level ϵ_{N+1} contributes both to A_{N-1} and B_{N+2} . Figure 3 shows the evolution of Ret and α for a specific series of couplings for U=0 (upper panel) and $U=60\Delta$ (lower panel), and $kT=\Delta/12$. We focus on four resonances (at integer values of V_g) with $\eta_1=\eta_2=-\eta_3=\eta_4=1$. For U=0 we have a phase lapse in the valley between the first and the second resonance (Ret becomes zero there) and no phase lapses between the others, as explained above. For interacting electrons we observe near resonance phase lapses (NR-PLs) due to the background terms which make the phase stay at $\alpha=\pi$ for almost all values of V_g , except near the resonances.

For the impurity-averaged correlations we define $C_t = \langle t(x,N)t^*(\bar{x},N+\delta N)\rangle/\sqrt{\langle |t(x,N)|^2\rangle\langle |t(\bar{x},N+\delta N)|^2\rangle}$ and $C_\alpha = \langle \cos\alpha(x,N)\cos\alpha(\bar{x},N+\delta N)\rangle$. The calculation of C_t follows [11]. The transmission amplitude [Eq. (6)] is given by $t(E) \sim V^L V^R \int d\omega \left[G_\omega^A(L,R) - G_\omega^R(L,R)\right] \times G_\omega^{\rm ret}(E,N,x)$ where $V^{L,R}$ describe the left and the right barrier. We note that this expression consists of a disorder-dependent (but interaction-independent) factor, and one, $G^{\rm ret}$, which includes the interaction (but not the disorder). One then readily obtains

$$C_t(x, N, x, N + \delta N)$$

$$= u \frac{x(1-x)}{\delta N} \left[\log \left(1 + \frac{\delta N}{xu} \right) + \log \left(1 + \frac{\delta N}{(1-x)u} \right) \right]$$
(8)

with $u = U/\Delta$. C_t decays slowly on a scale of $\delta N \sim U/\Delta$. We also observe the following: (i) For the non-interacting case C_t falls abruptly to zero for $\delta N = 1$. (ii) The results for the toy model and for a more realistic model, where ϵ_j and $V_j^L V_j^{R*}$ are obtained from diagonalizing random matrices, agree well, implying that the

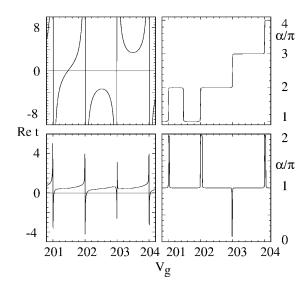


FIG. 3. Ret (left) and phase (right) for a specific sequence of resonances, for U=0 (upper panels) and $U=60\Delta$ (lower panels).

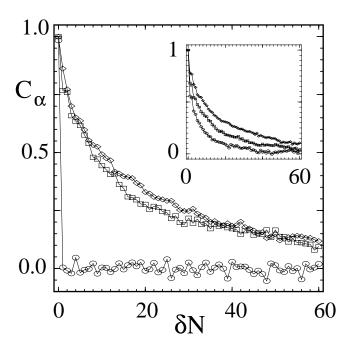


FIG. 4. Correlation function C_{α} vs the valley number for $kT = \Delta/12$. Interacting electrons (boxes and diamonds, $U = 50\Delta$, $x_1 = x_2 = 0.5$) show strong correlations; noninteracting electrons (circles, $x_1 = x_2 = 0.25$) do not. Toy model statistics (boxes) agrees well with random matrix model statistics (diamonds). Inset: Increasing the interaction increases the correlations (upper curve: $U = 50\Delta$, middle: $U = 25\Delta$, lower: $U = 12\Delta$).

correlations are fairly insensitive to the way randomness enters. These two remarks apply for C_{α} which is calculated numerically. Figure 4 shows C_{α} vs the distance in valleys δN for $kT=\Delta/12$. Noninteracting electrons forget about their phase already after one valley. In contrast, for interacting electrons we observe a slow decrease of C_{α} , showing that information about the phase in valley N is transferred to valley $N+\delta N$ [12]. The inset of Fig. 4 shows the decay of C_{α} for different values of the interaction. The decay is slower for stronger interaction.

To summarize we have proposed here a generic mechanism which gives rise to strong transmission phase correlations. Our approximate sum rule is subjected to errors which occur at a frequency $\sim U/\Delta$. Our mechanism involving a large number of small random contributions is conceptually different from recent models [6,13] which have utilized particularly strongly coupled levels and which depend on rather specific geometric arrangements.

Comparing our analysis to experiments [2] we note that in the latter $\Delta > \Gamma > kT$, implying that the resolution near the resonance may not be sufficient to observe NRPL directly [14]. A crucial test of our theory would be to go to small dots with small U/Δ , or, even better [15] to use other gates to scramble the dot as we sweep from one

valley to another, suppressing correlations among valleys. This should lead to a breakdown of our sign sum rule.

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