Spin and e-e interactions in quantum dots: Leading order corrections to universality and temperature effects

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We study the statistics of the spacing between Coulomb blockade conductance peaks in quantum dots with large dimensionless conductance \( g \). Our starting point is the “universal Hamiltonian”—valid in the \( g \to \infty \) limit—which includes the charging energy, the single-electron energies (described by random matrix theory), and the average exchange interaction. We then calculate the magnitude of the most relevant finite \( g \) corrections, namely, the effect of surface charge, the “gate” effect, and the fluctuation of the residual e-e interaction. The resulting zero-temperature peak spacing distribution has corrections of order \( \Delta / \sqrt{g} \). For typical values of the e-e interaction (\( r_s \sim 1 \)) and simple geometries, theory does indeed predict an asymmetric distribution with a significant even/odd effect. The width of the distribution is of order \( 0.3\Delta \), and its dominant feature is a large peak for the odd case, reminiscent of the \( \delta \)-function in the \( g \to \infty \) limit. We consider finite temperature effects next. Only after their inclusion is good agreement with the experimental results obtained. Even relatively low temperature causes large modifications in the peak spacing distribution: (a) its peak is dominated by the even distribution at \( k_B T \sim 0.3\Delta \) (at lower \( T \) a double peak appears); (b) it becomes more symmetric; (c) the even/odd effect is considerably weaker; (d) the \( \delta \)-function is completely washed-out; and (e) fluctuation of the coupling to the leads becomes relevant. Experiments aimed at observing the \( T = 0 \) peak spacing distribution should therefore be done at \( T < 0.1\Delta / k_B \) for typical values of the e-e interaction.

I. INTRODUCTION

The Coulomb Blockade (CB) of electron tunneling is one of the most studied effects in quantum dots (QDs). It allows one to probe quantum interference effects in both the wavefunction and the energy of interacting electrons. The main way in which the latter has been probed is through the spacing between adjacent CB conductance peaks. A satisfactory explanation for the observed CB peak spacing distribution (PSD) has, however, remained elusive. In this paper we first focus on the \( T = 0 \) PSD and find its shape for quantum dots containing a few hundred electrons. We then turn to the effect of temperature, showing that it is surprisingly large. In that case, electron transport through the QD is blocked—a double peak appears); (b) it becomes more symmetric; (c) the even/odd effect is considerably weaker; (d) the \( \delta \)-function is completely washed-out; and (e) fluctuation of the coupling to the leads becomes relevant. Experiments aimed at observing the \( T = 0 \) peak spacing distribution should therefore be done at \( T < 0.1\Delta / k_B \) for typical values of the e-e interaction.

Within the CI model, electrons fill the states of the QD in an “up-down” scheme due to the spin degeneracy. This implies a strong even/odd effect on the PSD. However, none of the experiments to date have shown such an effect—though a weak even/odd effect was observed, suggesting that spin plays a more active role. Furthermore, the observed PSD presents a Gaussian-like shape (with broader non-Gaussian tails), which contradicts the expected Wigner-Dyson distribution from random matrix theory. Finally, the magnitude of the width of the PSD was questioned. Early experiments found it scaled with \( E_C \), which is much bigger than the predicted value, \( \sim \Delta \), the single-particle mean level spacing. More recent experiments, however, showed that it is indeed of order \( \Delta \).

The search for an explanation to these discrepancies triggered several theoretical works over the last years. Initially, by the earlier experiments it was suggested that GS fluctuations were dominated by the e-e interaction itself. Therefore, a completely different approach—involving non-perturbative methods such as self-consistent Hartree-Fock or exact diagonalization—was required. On the other hand, based on the fact that a typical QD contains a large number of electrons, \( N \gg 1 \), it was argued that they should be described as “good” metals. This implies that the residual e-e interactions (i.e., those beyond \( E_C \)) are weak and can be added to the CI model perturbatively. We shall take the latter approach and show that it provides a good description of the
The small parameter in this perturbative approach is \( g = E_b / \Delta \) with \( q = E_b / \Delta \) the dimensionless conductance and \( E_b \) the Thouless energy (approximately \( h \) times the inverse time of flight). The condition for the QD to be a good conductor is \( g \lesssim \sqrt{N} \gg 1 \). Interaction corrections are classified by their order in \( g \) and successively added to the CI Hamiltonian. It then becomes clear why the CI model is wrong: there is a zero-order correction—i.e., a correction of order \( \Delta \)—namely, the average exchange interaction \( \tilde{S}^z \). Although this is a small correction to the total energy of the QD—and so the perturbative approach is justified—it is crucial for properties, like the CB peak spacing, that are sensitive to single levels in the QD. The zero-order Hamiltonian—hereafter called the constant exchange and interaction (CEI) model—is given by:

\[
\hat{H}_{\text{CEI}} = \sum_{\alpha,\sigma} \varepsilon_\alpha \hat{n}_{\alpha,\sigma} + E_C (\hat{n} - N)^2 - J_S \tilde{S}^2
\]

where \( \{ \varepsilon_\alpha \} \) are the single-electron energies, \( N = C_g V_g / e \) describes the capacitive coupling to the control gate, \( C_g \) is the dot-gate capacitance, \( \tilde{S} \) is the total spin operator, and \( J_S \) is the exchange constant. The difference between the CEI and CI models is the additional term proportional to \( \tilde{S}^2 \). Because it sometimes leads to a GS with \( S = 1 \), the simple “up-down” filling scheme breaks down. The corresponding PSD is completely different from the CI model result (see Ref. 29 for a plot). In fact, a GS with \( S = 1 \) has been experimentally observed very recently. The PSD resulting from the CEI model is still, however, in poor agreement with the data.

Most of the work so far has concentrated on the calculation of higher order corrections to the Hamiltonian. The most important ones are: (1) the “scrambling” of the spectrum when adding an electron to the QD, (2) the fluctuation of the diagonal matrix element of the \( e-e \) interaction and finally, not related to the \( e-e \) interaction, (3) the change in the single-electron energies when the gate voltage is swept. Surprisingly, although these corrections have been discussed previously in the literature, an explicit calculation of the PSD including all of them has not been done—note however that Ref. 29 included the first two. Here we present results that include all three effects and show that the scrambling and gate effects, though dominant, are much smaller than usually assumed in the literature. We also show that the fluctuation of the off-diagonal matrix elements introduces a small correction—in the regime relevant for the experiments—and can be disregarded in the calculation of the PSD. Despite the substantial improvement these corrections introduce, the disagreement with the experimental results persists.

Very recently, it was pointed out that there is a simple effect that has not been taken into account: finite temperature— we should mention that temperature effects have been discussed in terms of spinless particles. In our previous paper, we showed that in the CEI model the temperature effects are more important than in the CI model and that they become significant even at \( k_B T \sim 0.1 \Delta \). Since most experiments were done in the regime \( k_B T \sim 0.3-0.5 \Delta \)—an exception is Ref. 13—our results are crucial for interpreting the experimental data. Here, we present those results in more detail and extend them. We show that, because of temperature, the fluctuation of the coupling to the leads strongly affects the PSD. It is not until temperature is introduced that good agreement with the experimental results is obtained. Furthermore, temperature introduces the biggest correction in the regime where most experiments were done so far and constitutes the main cause of smoothing of the PSD. Consequently, lower temperature experiments are required in order to observe the actual ground state PSD.

The rest of the paper is organized as follows: in Section II we review the arguments that lead to the CEI model. The leading order corrections to this model are introduced in Section III. We calculate the contribution of the off-diagonal terms of the \( e-e \) interaction and the magnitude of the scrambling effect in Section IV and V respectively. Numerical results for the \( T = 0 \) PSD, including all the corrections, are presented in Section VI. We introduce the effect of finite temperature in Section VII. Finally, we conclude in Section VIII.

### II. THE CEI MODEL

At low temperature and low bias, only a few energy levels around the Fermi energy \( (E_F) \) are involved in the transport process. Consequently, an effective Hamiltonian \( \hat{H}_{\text{QD}} \) capable of describing the QD in that energy window is all that is needed. When considering single-particle properties of chaotic (or diffusive) QDs, it is well-known that \( \hat{H}_{\text{QD}} \) can be described by random matrix theory (RMT) provided that \( g \gg 1 \). This approach is valid within an energy window up to the Thouless energy \( E_b \). The single-particle Hamiltonian is then “universal”, i.e. it only depends on the symmetry of the problem—broken time-reversal symmetry is assumed throughout the paper—and, of course, the energy scale \( \Delta \).

This approach has proved to be quite successful for understanding the role of mesoscopic fluctuations in transport properties of QD (see Refs. 3 and 57 for reviews).

On the other hand, the treatment of the \( e-e \) interaction is more subtle. A proper description requires taking into account the screening of the bare Coulomb interaction provided by the electrons beyond \( E_b \). If the interactions are not so strong, i.e. if the gas parameter \( r_s \) is small, the screening can be calculated using the random phase approximation. In that case, the screened potential reads:

\[
V_{SC}(r_1, r_2) = \frac{e^2}{C} + V_{TF}(r_1) + V(r_1)\Delta + V(r_2)\Delta
\]

where \( C \) is the capacitance of the QD, \( V_{TF}(r) \) is the Thomas-Fermi screened potential and \( V(r)\Delta \) is a finite-size screened potential—its specific form and origin will be discussed in Section III. Here and throughout this paper we consider two-dimensional (2D) quantum dots. The last three terms in Eq. 2 are of order \( \Delta \) and so much smaller than the first term.
This leads to the following Coulomb interaction Hamiltonian

\[ \hat{H}_{\text{int}} = E_C (\hat{n}^2 - \hat{n}) + (\hat{n} - 1) \sum_{\alpha, \sigma} \varepsilon^\dagger_{\alpha, \sigma} c_{\alpha, \sigma} \chi_{\alpha, \beta} \]

\[ + \frac{1}{2} \sum_{\alpha, \beta, \gamma, \delta} H_{\alpha, \beta, \gamma, \delta} c_{\delta, \sigma}^\dagger c_{\gamma, \sigma}^\dagger c_{\beta, \sigma} c_{\alpha, \sigma} \]

(3)

where

\[ H_{\alpha, \beta, \gamma, \delta} = \int dr_1 dr_2 \Psi^\dagger_{\beta}(r_1) \Psi^\dagger_{\delta}(r_2) \times V_{\text{TF}}(r_1 - r_2) \Psi_{\beta}(r_2) \Psi_{\delta}(r_1) \]

\[ + \frac{1}{2} \int dr_1 dr_2 \Psi^\dagger_{\beta}(r_1) \Psi^\dagger_{\delta}(r_2) \times V_{\text{TF}}(r_1 - r_2) \Psi_{\beta}(r_2) \Psi_{\delta}(r_1) \]

(4)

\[ \chi_{\alpha, \beta} = \Delta \int dr V(r) \Psi^\dagger_{\alpha}(r) \Psi^\dagger_{\beta}(r) \] and \( \Psi_{\alpha}(r) \) is the eigenfunction of the single-electron Hamiltonian with eigenvalue \( \varepsilon_{\alpha} \). Fluctuations of the wavefunctions cause both \( H_{\alpha, \beta, \gamma, \delta} \) and \( \chi_{\alpha, \beta} \) to fluctuate. However, since both matrix elements are defined as integrals over the QD’s area, \( A \), one could expect the main contribution to come from their mean value due to self-averaging. It turns out that this is indeed the case and that the parameter that controls the relative importance of the fluctuations is \( 1/g \) (or equivalently \( 1/k_F \sqrt{A} \)). This suggests we can expand \( \hat{H}_{\text{int}} \) in powers of \( 1/g \) and keep only the dominant terms.

The zeroth-order term \( (g \to \infty) \) in this expansion corresponds to taking the mean value of the matrix elements,

\[ \langle H_{\alpha, \beta, \gamma, \delta} \rangle^{(0)} = J' \delta_{\alpha, \delta} \delta_{\beta, \gamma} + J_S \delta_{\alpha, \gamma} \delta_{\beta, \delta} \]

(5)

where \( J' = A^{-2} \int dr_1 dr_2 \Psi^\dagger_{\beta}(r_1) \Psi^\dagger_{\delta}(r_2) \times V_{\text{TF}}(r_1 - r_2) \sim A/2 \) and

\[ J_S = \frac{1}{A} \int dr V_{\text{TF}}(r) J^2(r) \]

(6)

is the exchange constant, \( J_0(x) \) is a Bessel function (2D case) and \( k_F \) is the Fermi wavevector. We shall see in Section II A that \( \langle \chi_{\alpha, \beta} \rangle = A/2 \delta_{\alpha, \beta} \). Introducing these mean values in Eq. (6) we obtain the “universal” part of the interaction Hamiltonian

\[ \hat{H}_{\text{int}}^{(0)} = E_C \hat{n}^2 - J_S \hat{S}^2 \]

(7)

where we have dropped terms linear in \( \hat{n} \) and redefine \( E_C \) to include all the terms proportional to \( \hat{n}^2 \). Here, \( \hat{S} = \sum_{\alpha, \sigma} \varepsilon^\dagger_{\alpha, \sigma} c_{\alpha, \sigma} \chi_{\alpha, \beta} \) is the total spin operator of the QD. Eq. (7) is the most general form of the interaction Hamiltonian compatible with RMT. Adding the coupling to the control gate gives the CEI model Hamiltonian [Eq. (8)].

Using the explicit expression for \( V_{\text{TF}}(r) \), we can rewrite \( J_S \) in terms of the gas parameter \( \var{r} \),

\[ J_S = \frac{r \Delta \text{Arcsec}(r \sqrt{2})}{\pi \sqrt{r^2 - 2}} \]

(8)

Note that \( J_S \leq \Delta/2 \) is a fixed quantity. Fluctuations in the spectrum of \( \hat{H}_{\text{CEI}} \) arise only from \( \{\varepsilon_{\alpha}\} \). This is a key point for understanding its GS: while in the CI model the levels are filled in an “up-down” scheme—which leads to a bimodal PSD—in the CEI model it is energetically favorable to promote an electron to a higher level and gain exchange energy whenever the spacing between the top two single-particle levels is smaller than \( 2J_S \) (\( N \) even). This is why the PSD is very different from the CI model result.

III. LEADING ORDER CORRECTIONS TO UNIVERSALITY

In the previous section we considered the simplest model for \( \hat{H}_{\text{QD}} \), which only takes the universal part of the residual interactions into account. Here, we include the next order corrections: (1) the “scrambling” of the spectrum when adding an electron to the QD, (2) the fluctuation of the diagonal part of the e-e interaction, and (3) the change in the single-electron energies when the gate voltage is swept. Although (2) is a correction of order \( \Delta/\sqrt{g} \) to the Hamiltonian, all three effects lead to corrections of order \( \Delta/\sqrt{g} \) to the spacing. We discuss now each of them in detail.

A. Scrambling

The scrambling effect [2] is caused by the presence of the potential \( V(r) \Delta \) in Eq. (2), which leads to the second term in Eq. (6). Its physical origin is quite simple. When an electron is added to the QD, the other electrons arrange themselves to screen the extra charge. That means that a charge \(-e/\kappa \) is pulled out to the boundaries of the QD. This extra charge creates an additional potential, \( V(r) \Delta \), for the electrons inside the QD. While in 3-D materials the charge is confined to a small region near the surface, in 2-D it is inhomogeneously distributed over the whole area of the QD.

It is straightforward to show that \( \langle \chi_{\alpha, \beta} \rangle = V \Delta \delta_{\alpha, \beta} \). The mean value thus does not introduce any correction to the CEI model—it should be added to \( E_C \). The correction comes only from the fluctuations of \( \chi_{\alpha, \beta} \). In particular, the main contribution (to the spacing) arises from \( \chi_{\alpha, \alpha} \), with \( \alpha \) the top level [3]. Its variance is given by,

\[ \text{var}(\chi_{\alpha, \alpha}) = \Delta^2 \int dr_1 dr_2 V(r_1) V(r_2) \langle |\Psi_{\alpha}^*(r_1) \Psi_{\alpha}(r_2)|^2 \rangle. \]

(9)

with \( V(r) = \bar{V}(r) - \bar{V} \).

With corrections of order \( 1/g \) included, the wavefunction correlation appearing in Eq. (9) is given by [3],

\[ A^2 \langle |\Psi_{\alpha}^*(r_1) \Psi_{\alpha}(r_2)|^2 \rangle = 1 + k(r_1, r_2) - k(r_1) - k(r_2) + k + \Pi_{\text{B}}(r_1, r_2) \]

(10)

with \( k(r_1, r_2) = J^2_3(k_F |r_1 - r_2|) \), \( k(r) = A^{-2} \int dr_1 k(r, r_1) \), and \( k = A^{-2} \int dr_1 dr_2 k(r_1, r_2) \). \( \Pi_{\text{B}}(r_1, r_2) \) is a classical propagator that contains the contributions of the trajectories that reach the boundary of the QD—it is therefore geometry dependent. The latter satisfies \( \int dr_1 \Pi_{\text{B}}(r_1, r_2) = 0 \) with \( i = 1 \) or 2. The second term in Eq. (10) corresponds to Berry’s result: on scales smaller than the system size \( \sqrt{A} \), the correlation of chaotic wavefunctions is giving by a random superposition of plane waves. The other terms involving \( k(r_1, r_2) \) properly account for the normalization of the wavefunctions.
After substituting (9) in (8) we get
\[
\text{var}(\chi_{\alpha,\alpha}) = \frac{\Delta^2}{A^2} \int dr_1 dr_2 \tilde{V}(r_1) \tilde{V}(r_2) k(r_1, r_2) + \frac{\Delta^2}{A^2} \int dr_1 dr_2 \tilde{V}(r_1) \tilde{V}(r_2) \Pi_B(r_1, r_2).
\]
(11)

For quantitative evaluation we consider the case of a ballistic circular disc with diffusive boundary conditions. For this system, we get
\[
\Pi_B(r_1, r_2) = \frac{1}{4\pi k_F} \sum_{q=1}^\infty \frac{4g^2-1}{4g^2} \left( \frac{r_1 r_2}{R^2} \right)^q \cos(q(\theta_1-\theta_2))
\]
(12)

where \( r_i = r_i(\cos \theta_i, \sin \theta_i) \). Thus the last term in (11) yields 0 exactly since the potential \( V(r) \) is isotropic (in the isolated dot case, see Section V). For a general geometry, the form of \( \Pi_B \) is not known, and there is no reason a priori to expect such a cancellation. We assume that the contribution of this term is of the same order as the first and that our final result for the var(\( \chi_{\alpha,\alpha} \)) is correct up to a factor 2\[4].

Since \( k(r_1, r_2) \approx 1/\pi k_F |r_1 - r_2| \), a simple dimensional analysis of the first term in Eq. (11) shows that it is proportional to \( \Delta^2/k_F \sqrt{A} \) so that
\[
\text{var}(\chi_{\alpha,\alpha}) = b_{00} \frac{\Delta^2}{g}.
\]
(13)

The same result is valid for var(\( \chi_{\alpha,\beta} \)). Again using the circular disc with diffusive boundaries for quantitative estimation we have \( E_{\alpha,\beta} = \hbar \gamma_1 v_F / R \) so that \( g = \gamma_1 k_F \sqrt{A}/2\sqrt{\pi} \) with \( \gamma_1 = 0.35 \). The approximate value of the geometry-dependent coefficient \( b_{00} \) is calculated in Section IV.

### B. Diagonal matrix elements

Recently, Ref. 29 has shown that the fluctuation of the diagonal terms of \( H_{\text{int}} \) leads to a correction to the spacing of the same order as the scrambling, despite the fact that the variance of the diagonal matrix elements is of order \( \Delta^2/g^2 \). The reason is that the correction due to these terms involves a sum over \( \approx g \) levels. To see this, let us first calculate the variance of the diagonal matrix elements. In the zero-range approximation, where the short-range screened potential is approximated by a \( \delta \)-function, \( V_{\text{TF}}(r) \approx \delta(r) \Delta A/2 \), it is given by
\[
\text{var}(M_{\alpha,\beta}) = \frac{\Delta^2}{4A^2} \int dr_1 dr_2 \left[ k(r_1 - r_2) + \Pi_B(r_1, r_2) \right]^2
\]
(14)

where \( M_{\alpha,\beta} = H_{\alpha,\beta,\beta,\alpha} - (H_{\alpha,\beta,\beta,\alpha})^{(0)} \) and \( k(r_1 - r_2) = k(r_1 - r_2) - k(r_1) - k(r_2) + k \). Using the full expression for \( V_{\text{TF}} \) leads to similar numerical results—in that case it is important to keep the correlation between the direct and the exchange terms. The dominant contribution in Eq. (14) comes from \( |k(r_1 - r_2)|^2 \)—the other terms are of the same order in \( 1/g \) but numerically much smaller—so
\[
\text{var}(M_{\alpha,\beta}) = \frac{3\Delta^2 \ln(4k_F \sqrt{A})}{4\pi} \frac{\ln g}{g^2} \Delta^2.
\]
(15)

For the double-diagonal matrix element, \( \text{var}(M_{\alpha,\alpha}) = 4 \text{var}(M_{\alpha,\beta}) \). Let us now consider the contribution of the fluctuation of the diagonal terms to the spacing corresponding to the transition \( 1/2 \to 0 \to 1/2 \).

\[
s_{\text{diag}} = \sum_{\beta \neq \alpha} \left( M_{\alpha+1,\beta} - M_{\alpha,\beta} \right). \tag{16}
\]

Neglecting the correlation between the different matrix elements, we get \( \text{var}(s_{\text{diag}}) \approx 2g \text{var}(M_{\alpha,\beta}) \propto \Delta^2 \ln g/g \). The contribution of these terms to the spacing fluctuations is, then, of the same order as the scrambling, namely \( \Delta^2/\sqrt{g} \).

A similar result can be obtained for all the different spin transitions except for \( 0 \to 1/2 \to 0 \). In that particular case \( s_{\text{diag}} = M_{1/2,1/2} \) and therefore \( \text{var}(s_{\text{diag}}) \propto \Delta^2/g^2 \). This is an exact result not related to the zero-range approximation for \( V_{\text{TF}} \). For this reason, the effect of the fluctuation of the diagonal terms on the \( \delta \)-function of the PSD is weak, though noticeable.

Diagonal terms produce fluctuations of the energy difference between the singlet and triplet states, \( E_{S=0} - E_{S=1} \). It is straightforward to verify that \( \text{var}(E_{S=0} - E_{S=1}) \approx 2g \text{var}(M_{\alpha,\beta}) \). Since the exchange contribution to this energy difference is \( 2J_S \), we can think of this as an effective fluctuation in \( J_S \). These fluctuations might lead to a change of the ground state in the cases where the triplet and singlet states are almost degenerate.

It is worth commenting that there is a correction of order \( 1/g \) to the mean value of the diagonal matrix elements. In the zero-range limit it is given by
\[
\langle H_{\alpha,\beta,\gamma,\gamma} \rangle^{(1/g)} = c_1 \frac{\Delta^2}{2g} (\delta_{\alpha,\delta} \delta_{\beta,\gamma} + \delta_{\alpha,\gamma} \delta_{\beta,\delta})
\]
(17)

with \( c_1 = 9A^{-1} \int dr \Pi_B(r, r) \). This correction can be included in the definition of \( E_C \) and \( J_S \) since it has the same structure as Eq. (5). For a ballistic disc, this introduces a correction of \( -0.008 \Delta \) in the latter.

Before closing this subsection we should point out that \( \langle M_{\alpha,\beta} \chi_{\alpha,\alpha} \rangle = O(1/g^2) \). In principle this also leads to a \( \Delta^2/\sqrt{g} \) correction to the spacing. Rough estimates suggest that it is numerically small, however, and so we neglect it.

### C. “Gate” effect

The two contributions we have discussed so far are usually regarded as intrinsic, in the sense that their origin is the e-e interaction of the particles in the QD itself. On the other hand, the effect of the gate voltage is usually associated with the distortion of the shape of the QD when the gate voltage is swept. Consequently, it appears that it could be
The correction to the confinement potential due to a change in the gate voltage is:

\[
\delta U(r) = -2E_G \delta N - \Delta \left[ V(r) \delta N + \sum_i V^{(i)}(r) \delta N_i \right]
\]

(18)

with \( \delta N = \sum_i \delta N_i \), \( \delta N_i = C_{ij}^\alpha \delta V_j^\alpha / e \) and \( \delta V_j^\alpha \) is the change of the electrostatic potential of the \( i \)-th gate. The potentials \( V(r) \) and \( V^{(i)}(r) \) are related to the solution of the electrostatic problem associated with the set of conductors (QD+gates)—see next section and Ref. [5] for more details. The former is the same potential that appears in Eq. (5) and causes the screening effect. It is clear then that a change in \( \delta N \) produces the same effect as a change of \( N \). This is reasonable since these two effects are opposite faces of the same electrostatic problem: a change of the electrostatic potential of the QD produces a non-uniform distribution of charge, which creates a change in the potential of the QD; vice versa, an extra charge must be distributed in the same way so that the potential of the QD is uniform. Eq. (18) leads to the following correction to the Hamiltonian:

\[
\hat{H}_\text{gate} = - \sum_{\alpha,\beta,\sigma} c_{\alpha,\sigma}^\dagger c_{\beta,\sigma} \left[ \delta N \hat{X}_{\alpha,\beta}^{\sigma} + \sum_i \delta N_i \hat{X}_{\alpha,\beta}^{i\sigma} \right]
\]

(19)

where \( \hat{X}_{\alpha,\beta}^{i\sigma} \) is defined in terms of \( V^{(i)}(r) \)—it is then clear that \( \text{var}(\hat{X}_{\alpha,\beta}^{i\sigma}) = h_{ii}\Delta^2 / g \), with \( h_{ii} \) a geometry dependent numerical coefficient.

Notice that the change in the shape of the QD can be associated with the last term in Eq. (19). For instance, if the potentials of two plunger-gates are swept in a way such that the potential of the QD is uniform, Eq. (19) leads to the following correction to the Hamiltonian:

\[
\hat{H}_\text{gate} = - \sum_{\alpha,\beta,\sigma} c_{\alpha,\sigma}^\dagger c_{\beta,\sigma} \left[ \delta N \hat{X}_{\alpha,\beta}^{\sigma} + \sum_i \delta N_i \hat{X}_{\alpha,\beta}^{i\sigma} \right]
\]

(19)

where \( \hat{X}_{\alpha,\beta}^{i\sigma} \) is defined in terms of \( V^{(i)}(r) \)—it is then clear that \( \text{var}(\hat{X}_{\alpha,\beta}^{i\sigma}) = h_{ii}\Delta^2 / g \), with \( h_{ii} \) a geometry dependent numerical coefficient.

Notice that the change in the shape of the QD can be associated with the last term in Eq. (19). For instance, if the potentials of two plunger-gates are swept in a way such that

\[
\delta N = \delta N_1 + \delta N_2 = 0 \text{ then the change of the confinement potential originates only from that term, and the effect of a change in the shape of the QD can be isolated.}
\]

Note, however, that this procedure actually tests only the difference between \( V^{(1)}(r) \) and \( V^{(2)}(r) \), which could be smaller that each one of them if the two gates are in similar positions with respect to the QD.

IV. OFF-DIAGONAL MATRIX ELEMENTS.

So far we have considered only the contribution of the diagonal terms of \( \hat{H}_\text{int} \). We found that although the fluctuation of each individual matrix element is of the order of \( \Delta / g \), the total contribution to the peak spacing is of order \( \Delta / \sqrt{g} \). This is a consequence of the addition of the \( \sim g \) different matrix elements that contribute to the spacing. Since in principle there are many more off-diagonal terms, one might wonder if their contribution can also add up and result in a significant one that should also be included. We show now that this is not the case.

The first correction to the GS energy due to off-diagonal terms appears in second order perturbation theory (the first order contribution is zero by definition)

\[
E_S^{(2)} = \sum_j \frac{|\langle \Psi_j | \hat{H}_\text{int} | \Psi_N \rangle|^2}{E_S^{(0)} - E_j^{(0)}}
\]

where \( |\Psi_N \rangle \) is the GS of the system (described by \( \hat{H}_\text{CB} \)) with \( N \) electrons and spin \( S \), and \( \{ |\Psi_j \rangle \} \) are the excited states.

Following Ref. [5], we rewrite the off-diagonal part of the Hamiltonian (5) as follows,

\[
\hat{H}_\text{int}^{\text{off}} = \sum_{\beta > \alpha, \gamma \geq \delta} u_{\alpha, \beta, \gamma, \delta} \left( c_{\delta, \gamma}^\dagger c_{\gamma, \delta}^\dagger c_{\beta, \gamma} c_{\alpha, \delta} + c_{\delta, \gamma}^\dagger c_{\gamma, \delta}^\dagger c_{\alpha, \gamma} c_{\beta, \delta} + \frac{1}{2} (c_{\delta, \gamma}^\dagger c_{\gamma, \delta}^\dagger c_{\beta, \gamma} c_{\alpha, \delta} + c_{\delta, \gamma}^\dagger c_{\gamma, \delta}^\dagger c_{\beta, \delta} c_{\alpha, \gamma}) \right)
\]

(20)

where \( u_{\alpha, \beta, \gamma, \delta} = H_{\alpha, \beta, \gamma, \delta} - H_{\alpha, \beta, \delta, \gamma} \)

The sum in Eq. (21) runs over all configurations in which the indices of \( c^\dagger \) and \( c \) are not fully paired (that is, the configurations not included in a Hartree-Fock treatment). From this form of the Hamiltonian, it is easy to see that \( \hat{H}_\text{int}^{\text{off}} \) conserves the total spin. The first term produces only triplet-transitions while the second only singlet-transitions. Because of that, the states coupled by \( \hat{H}_\text{int}^{\text{off}} \) have the same spin. Then, the energy denominator that appears in Eq. (21) involves differences between single-electron energies. The spin rotational invariance of \( \hat{H}_\text{int}^{\text{off}} \) also implies that the second order correction to the energy is the same for all the states in a given spin-multiplet (i.e. the states with different \( S_z \)). Therefore, we can use the one with the maximum value of \( S_z \), the simplest state, throughout our calculations.

The difficulty in calculating \( E_S^{(2)} \) lies in recognizing which terms have to be added coherently, that is to say, which terms lead to the same final state \( |\Psi_N \rangle \). This complication arises because of: (i) the indices in Eq. (21) might be partially paired,
so terms within each of the two main terms do not necessarily produce orthogonal states, or (ii) non-trivial states, like the \( S = 1 \) state, can lead to the same final state under the action of any of the two main terms in Eq. (21) for particular values of the indices. In order to avoid the first problem, we explicitly take into account all the possible pairing of the indices and rewrite Eq. (21) as

\[
\hat{H}_{\text{int}} = \hat{H}_A + \hat{H}_B + \hat{H}_C
\]

with

\[
\hat{H}_A = \sum_{\alpha,\beta,\gamma} \sum_{\sigma} \left[ u_{\alpha,\beta,\gamma,\sigma} \hat{n}_{\alpha,\sigma} \hat{c}_{\gamma,\sigma} \hat{c}_{\beta,\sigma} + \frac{1}{2} (u_{\alpha,\beta,\gamma,\sigma} + a_{\alpha,\beta,\gamma,\sigma}) \hat{n}_{\alpha,\sigma} \hat{c}_{\gamma,\sigma} \hat{c}_{\beta,\sigma} + \frac{1}{2} (u_{\alpha,\beta,\gamma,\sigma} - a_{\alpha,\beta,\gamma,\sigma}) \hat{n}_{\alpha,\sigma} \hat{c}_{\gamma,\sigma} \hat{c}_{\beta,\sigma} \right] + \sum_{\alpha,\beta} \frac{1}{2} (a_{\alpha,\beta,\beta,\beta} + a_{\beta,\alpha,\beta,\beta}) \hat{n}_{\beta,\sigma} \hat{c}_{\beta,\sigma} \hat{c}_{\beta,\sigma} \hat{c}_{\alpha,\sigma}.
\]

(24)

\[
\hat{H}_B = \sum_{\alpha,\gamma} \frac{1}{2} a_{\alpha,\alpha,\gamma,\gamma} \hat{c}_{\gamma,\uparrow} \hat{c}_{\gamma,\uparrow} c_{\alpha,\downarrow} c_{\alpha,\downarrow} + \sum_{\alpha,\gamma,\delta} \frac{1}{2} a_{\alpha,\alpha,\gamma,\delta} \left( \hat{c}_{\gamma,\uparrow} \hat{c}_{\delta,\uparrow} - \hat{c}_{\delta,\uparrow} \hat{c}_{\gamma,\uparrow} \right) c_{\alpha,\downarrow} c_{\alpha,\downarrow} + \sum_{\gamma,\beta,\alpha} \frac{1}{2} a_{\beta,\gamma,\beta,\gamma} \hat{c}_{\beta,\uparrow} \hat{c}_{\beta,\uparrow} \left( \hat{c}_{\gamma,\downarrow} c_{\alpha,\downarrow} - \hat{c}_{\gamma,\downarrow} c_{\alpha,\downarrow} \right)
\]

(25)

and \( \hat{H}_C \) as in Eq. (21) but with all the indices being different. Here, none of the remaining indices are paired and \( \sigma = -\sigma \). Notice that \( \hat{H}_A \) contains contributions from both terms in Eq. (21).

In general, the eigenstates of \( \hat{H}_{\text{CEI}} \) are a superposition of Hartree-Fock states. However, because \( S^2 \) and the single particle Hamiltonian commute, they can be classified by their occupation numbers \( \{n_{\alpha}\} \). For each configuration with \( N_s \) singly occupied levels, there are \( 2^{N_s} \) states which have different values of \( S \) and \( S_z \). It is worth mentioning that for \( N_s \geq 3 \), the values of \( S \) and \( S_z \) are not enough to specify a given eigenstate—instance, for \( N_s = 3 \), there are two orthogonal sets of states with \( S = \frac{1}{2} \). The determination of the precise form of the spin eigenstates in terms of the HF states is not a trivial task. Nevertheless, for our purpose, it is sufficient to notice that in order to add coherently two terms must lead to final states with the same occupation numbers. With this in mind, it is straightforward to check that \( \hat{H}_A, \hat{H}_B \) and \( \hat{H}_C \) add incoherently. In analyzing each of them however, we must proceed in a case by case basis.

At present, we are not aware of any simple method for evaluating Eq. (20) for an arbitrary state \( |\Psi_S^N\rangle \). However, it is sufficient for our purpose to calculate the correction for the cases \( S = 0, \frac{1}{2} \) and 1 since those are the most probable values of the spin for typical values of the e-e interaction. As an example, let us discuss the \( S = 0 \) case in detail. In this case, \( |\Psi_S^{N=0}\rangle \) has only doubly occupied levels (up to \( \hat{E}_0 \)). It is easy to see that the last two terms of \( \hat{H}_A \) give zero when applied on \( |\Psi_S^{N=0}\rangle \). The remaining terms of \( \hat{H}_A \) give,

\[
\hat{H}_A |\Psi_S^{N=0}\rangle = \sum_{\beta,\gamma} \left( \sum_{\alpha} \frac{1}{\sqrt{2}} (3u_{\alpha,\beta,\gamma,\alpha} + a_{\alpha,\beta,\gamma,\alpha}) \right) \frac{c_{\beta,\sigma}^\dagger c_{\gamma,\sigma}^\dagger + c_{\beta,\sigma}^\dagger c_{\gamma,\sigma}}{\sqrt{2}} |\Psi_S^{N=0}\rangle
\]

(26)

Note that the sum over \( \alpha \) does not affect the final states—this is an example of terms that add coherently—while each pair \( \{\beta, \gamma\} \) leads to a different final state. The factor \( \sqrt{2} \) was introduced to keep the final state properly normalized. Similarly, it is easy to check that each of the terms in \( \hat{H}_B \) and \( \hat{H}_C \) lead to orthogonal states. Adding up all the contributions, we finally get the following expression,

\[
E_S^{(2)} = \sum_{\beta,\gamma} \left( \sum_{\alpha} \frac{3|u_{\alpha,\beta,\gamma,\alpha} + a_{\alpha,\beta,\gamma,\alpha}|^2}{2(\varepsilon_\beta - \varepsilon_\gamma)} \right) + \sum_{\beta,\alpha,\gamma,\delta} \frac{3|u_{\alpha,\beta,\gamma,\delta}|^2 + |a_{\alpha,\beta,\gamma,\delta}|^2}{\varepsilon_\alpha + \varepsilon_\beta - \varepsilon_\gamma - \varepsilon_\delta} \left( 1 - \frac{\delta_{\beta,\gamma}}{2} \right) \left( 1 - \frac{\delta_{\beta,\delta}}{2} \right)
\]

(27)

where \( \alpha \) and \( \beta \) (\( \gamma \) and \( \delta \)) refer to occupied (empty) levels. Notice that the first (coherent) term is absent in Ref. [5]. Following a similar procedure, we have obtained expressions for \( S = \frac{1}{2} \) (see Appendix) and \( S = 1 \) which are too cumbersome to be presented here. In those cases, however, the presence of single occupied levels introduces some complications, and special care must be taken with the terms in which any of the indices correspond to one of these levels. It is also important to properly take into account the symmetry properties of the matrix elements, \( H_{\alpha,\beta,\gamma,\delta} = H_{\beta,\gamma,\alpha,\delta} \), as it affects the variance of \( u_{\alpha,\beta,\gamma,\delta} \) and \( a_{\alpha,\beta,\gamma,\delta} \). Note that in the particular case of the zero-range interaction limit, \( u_{\alpha,\beta,\gamma,\delta} = 0 \) and \( a_{\alpha,\beta,\gamma,\delta} = 2H_{\alpha,\beta,\gamma,\delta} \).

We calculate \( E_S^{(2)} \) numerically in the zero-range limit. We first evaluate the correction to the spin gap, \( \Delta_S = E_S^{(2)} - E_S^{(2)} = 1 \). We find that both \( \langle \Delta_S \rangle \) and \( \text{rms}(\Delta_S) \) are of order \( \Delta/g \) which, being a higher order correction, can be neglected. Nevertheless, we checked that for \( N = 500 \), \( \text{rms}(\Delta_S) \) is \( \sim 4 \) times smaller than the correction introduced by the diagonal terms. Therefore, we ignored any effect of the off-diagonal terms in the occupation of the states. This allows us to simply evaluate the correction to the spacing as \( s_{\text{aff}} = E_{S+1}^{(2)} - E_{S-1}^{(2)} - E_{N,1,0,0}^{(2)} \). We find that \( |s_{\text{aff}}| \propto \Delta^2/g^2 \) and so can also be neglected. An explicit evaluation for \( N = 500 \) gives \( \text{rms}(s_{\text{aff}}) = 0.016\Delta \) which is much smaller than the fluctuation introduced by the diagonal terms. The latter result corresponds to a generic transition, while for the special case \( 0 \rightarrow \frac{1}{2} \rightarrow 0 \) we get \( \text{rms}(s_{\text{aff}}) = 0.007\Delta \).
V. MAGNITUDE OF SCRAMBLING EFFECT

As we mentioned in the previous section, the origin of the potential \( V(r) \) in Eq. (3) is the screening charge \(-e/\kappa\). Although it has been known for a while that this leads to a correction of order \( \Delta/\sqrt{g} \) to the Hamiltonian, \( \text{var}(X_{\alpha,\beta}) = b_{00}\Delta^2/g \), a realistic estimate of the magnitude of \( b_{00} \) is still lacking. This is particularly important since the effect of the scrambling on the PSD goes in the right direction, i.e., it can lead to Gaussian-like distribution if it is strong enough. Here, we show that this has been overestimated in the literature and that scrambling is not able by itself to explained the experimental results.

The evaluation of \( b_{00} \) for actual geometries is quite difficult. The reason is that it involves finding the solution of the electrostatic field for a set of conductors in a particular geometry. Following Ref. [8] we write

\[
V(r) = \frac{A\kappa}{8\pi\varepsilon} \int d\mathbf{r}_2 \partial_2^\dagger \partial_2^\ddagger D(r, r_2) \tag{28}
\]

where \( \partial^\dagger_2 = \partial_{z_2} \), \( z \) is the axis perpendicular to the dot, \( D(r_1, r_2) \) is the Green function of the electrostatic problem outside the QD including the gates,

\[
\nabla_2^2 D(r, r_2) = -\delta(r-r_2), \quad D(r, r_2)|_{r \in S} = 0 \tag{29}
\]

with \( S \) the conducting surfaces and

\[
C = \frac{\kappa}{4\pi} \int d\mathbf{r}_1 d\mathbf{r}_2 \partial_2^\dagger \partial_2^\ddagger D(r_1, r_2) \tag{30}
\]

is the total capacitance of the QD. Eq. (28) has a very clear physical interpretation if we notice that

\[
\phi(r) = -\frac{e}{C} \int d\mathbf{r}_2 \partial_2^\dagger \partial_2^\ddagger D(r, r_2) \tag{31}
\]

is the electrostatic potential outside the QD with \( \phi(r)|_{r \in QD} = -e/C \) and \( \phi(r) = 0 \) over the gate electrodes. Then,

\[
V(r) = -\frac{A\kappa}{2\varepsilon} \sigma(r) \tag{32}
\]

with

\[
\sigma(r) = \frac{1}{4\pi} \partial_2^\ddagger \phi(r) \tag{33}
\]

the surface charge density in the QD associated with electrostatic potential \( \phi(r) \). Using Eq. (31), it is straightforward to show that \( Q = \int d\mathbf{r} \phi(r) = -e/\kappa \); note that this implies \( V = \frac{1}{2} \). Introducing Eq. (29) in Eq. (11) and using the fact that \( k(r_1, r_2) \approx 1/\pi k_F|r_1 - r_2| \) we get

\[
\text{var}(X_{\alpha,\beta}) = \frac{\Delta^2}{4\pi k_F^2 \sqrt{A}} \left[ \frac{1}{A^2} \int d\mathbf{r}_1 d\mathbf{r}_2 \frac{\partial_2^\dagger \partial_2^\ddagger D(r_1, r_2)}{|r_1 - r_2|} + \frac{\sqrt{A}}{Q^2} \int d\mathbf{r}_1 \left( \frac{\sigma(r_1)}{A} - \frac{2Q}{A} \phi'(r_1) \right) \right] \tag{34}
\]

where

\[
\phi'(r_1) = \int d\mathbf{r}_2 \frac{\sigma(r_2)}{|r_1 - r_2|} \tag{35}
\]

is the potential due to the surface charge in the QD. Let us now consider the different cases.

A. Isolated dot

In this case, the only charge in the system is \( \sigma(r) \) and the electrostatic potential \( \phi'(r) \) is constant over the QD surface, \( \phi'(r) = \phi(r) = -e/C \). This allow us to readily obtain

\[
\text{var}(X_{\alpha,\beta}) = \frac{\Delta^2}{4\pi k_F^2 \sqrt{A}} \left( \alpha - \frac{\sqrt{A\kappa}}{C} \right), \tag{36}
\]

with \( \alpha = A^{-\frac{3}{2}} \int d\mathbf{r}_1 d\mathbf{r}_2 (|r_1 - r_2|)^{-1} \). Notice that no particular geometry has been assumed so far. The first term in the parenthesis can be calculated numerically for arbitrary geometries. The second, however, requires the calculation of the capacitance. In the case of an ellipsoidal QD[4]

\[
\sqrt{\frac{A\kappa}{C}} = \sqrt{\frac{b}{a}} \int_{-1}^{1} F(\arcsin x, 1, \frac{1}{x^2}), \quad x = \sqrt{1 - \frac{b}{a} \frac{1}{2}} \tag{37}
\]

where \( a (b) \) is the length of the long (short) axis and \( F(\phi, m) \) is the elliptic integral of the first kind. For \( a/b \approx 1 - 3 \) we get \( b_{00} \approx 0.002 \). It is clear then that \( \text{rms}(X_{\alpha,\beta}) \approx 0.04 \Delta/\sqrt{g} \) is smaller than usually assumed. In fact, for \( N = 500 \), this value corresponds to \( \delta x = \sqrt{b_{00}/g} = 0.018 \) in the parametric approach to the scrambling, about a factor of 10 less than taken in Refs. [24] and [33].

B. Dot with gates

Since experiments are certainly done in the presence of gate electrodes, a careful calculation should take them into account. Looking at Eq. (34), it is tempting to simply replace \( C \) by its experimental value. However, the above calculation is only valid for an isolated QD, as we explicitly assumed that \( \sigma(r) \) was the only charge in the systems. For a real QD, the induced charge on the gates has to be considered. Then, \( \phi(r) = \phi'(r) + \phi''(r) \) where \( \phi''(r) \) is the potential created by the induced charge on the gates. Defining \( \phi'' = A^{-1} \int d\mathbf{r} \phi''(r) \) and \( \beta = (Q\phi'')^{-1} \int d\mathbf{r} \phi'(r) \phi''(r) \) we find

\[
\text{var}(X_{\alpha,\beta}) = \frac{\Delta^2}{4\pi k_F^2 \sqrt{A}} \left( \alpha - \frac{\sqrt{A\kappa}}{C} \left[ 1 + (2 - \beta) \phi'' \right] \right) \tag{38}
\]

Notice that the value of the ratio \( \sqrt{A\kappa}/C \) can now be obtained from the experimental data since \( C \) is the capacitance for the actual geometry.

Since \( \beta \sim 1 \) and \( \phi'' > 0 \) (the sign of the induced charge is the opposite of \( Q \)), it is evident that using the isolated dot
result [Eq. (36)] gives an upper limit to \( \text{var}(\mathcal{X}_{\alpha,\beta}) \) when evaluated with the experimental parameters. An estimate of \( \tilde{\phi}'' \) is obtained as follows. Let \( Q_i \) be the charge of the \( i \)-th gate, then \( \tilde{\phi}'' \sim \sum_i Q_i / d_i \kappa \), with \( d_i \) the distance between the centers of charge of the QD and the \( i \)-th gate. Since \( Q_i = -C_g^i (-e / C) \), where \( C_g^i \) is the dot-\( i \)-th gate capacitance, it turns out that \( \tilde{\phi}'' / (e / C) \sim \sum_i C_g^i / d_i \kappa \). Then,

\[
\frac{\sqrt{A \kappa}}{C} \frac{\tilde{\phi}''}{e / C} \sim 0.5 \frac{\sqrt{A}}{d}
\]

(39)

where we used that typically \( \sum_i C_g^i / C \sim 0.5 \) and denote by \( d \) the average distance between the center of the dot and the gates. For the data of Ref. [3] we estimate \( b_{00} \sim 0.005 \) with an upper limit of 0.01; thus, even with gate effects included, our estimate is smaller than values used previously [4,5].

VI. GROUND STATE PEAK SPACING DISTRIBUTION

We now use numerics for the evaluation of the PSD. At \( T = 0 \) (temperature effects will be discussed in the next section) the peak spacing is given by

\[
s_N = \left( E_{GS}^N(N') - E_{GS}^N(N) \right) - \left( E_{GS}^N(N) - E_{GS}^{N-1}(N) \right)
\]

(40)

where \( E_{GS}^N(N) \) is the GS energy of the QD with \( N \) electrons excluding the charging energy term and \( N' \) is the corresponding gate voltage. Including all the leading order corrections to the CEI model, the Hamiltonian reads

\[
\hat{H}_{\text{QD}} = \hat{H}_{\text{CEI}} + \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} \text{diag} \left( H_{\alpha,\beta,\gamma,\delta} \right) c_{\alpha,\sigma}^\dagger c_{\gamma,\sigma}^\dagger c_{\beta,\sigma} c_{\delta,\sigma} + \sum_{\alpha,\beta,\gamma} \left( (\hat{n} - N) \mathcal{X}_{\alpha,\beta} + \delta \mathcal{N} \mathcal{X}_{\alpha,\beta} \mathcal{X}_{\gamma,\beta} \right)
\]

(41)

where the variance of \( H_{\alpha,\beta,\gamma,\delta} \) and \( \mathcal{X}_{\alpha,\beta} \) are given by Eq. (15) and Eq. (16), respectively. Their mean values are included in the definition of \( E_C \) and \( J_S \), so that \( \langle H_{\alpha,\beta,\gamma,\delta} \rangle = \langle \mathcal{X}_{\alpha,\beta} \rangle = 0 \). The second term in Eq. (41) includes only the diagonal terms of the residual interaction, and \( \delta \mathcal{N} \) is taken with respect to some fixed state, for instance the state with \( N \) electrons. The GS energies were obtained by minimizing the energy with respect to the occupation numbers for \( N - 1, N, N + 1, \) and \( N + 2 \) (and the corresponding \( N', N'' \), and \( N''' \)). We only kept two consecutive spacings for each realization of the single-particle Hamiltonian. It is worth mentioning again that Eq. (41) is defined in a window up to \( E_{\text{th}} \), so that only \( g \) levels were considered.

The parameters we use are: (1) \( g = 0.38 \sqrt{N/2} \) (which corresponds to a disc geometry) [14,15] (2) the upper limit for the value of \( b_{00} \sim 0.01 \), and (3) \( b_{11} = b_{00} \). Only transitions with \( |\delta \mathcal{N}| = 1 \) were taken into account since in the absence of spin-orbit interaction (or if it is small), the transitions where the change in the GS spin is bigger than \( 1 \), appear as “missing” peaks in the conductance and are not included in the experiment.

Numerical results for \( N = 200, 500, \) and 1000 are shown in Fig. 1. The horizontal axis corresponds to \( s_N - J_S / 2 \), so that the origin agrees with the Hartree-Fock result of Ref. [2].

Corrections to the CEI model clearly smear-out all the sharp features of the PSD. The former \( \delta \) function (see inset in Fig. 1) is now a finite peak but still constitutes the dominant feature

![FIG. 1: Top panel: Ground state peak spacing distribution obtained from Eq. (14) with \( N = 500 (g \approx 6) \) and \( J_S = 0.28 \Delta (r_s = 1) \). The solid (dashed) line correspond to \( N \) odd (even). The origin of the horizontal axis corresponds to \( s_N = J_S / 2 \). The CEI model result is included in the inset for comparison. Note that all the sharp features, including the \( \delta \) function, are washed-out but the long tail for large spacing persists in the even case. Bottom panel: Comparison of the even (left) and odd (right) distributions for \( N = 200 \) (solid line) and \( N = 1000 \) (dashed line). Clearly, residual effects are stronger for \( N \) odd.]

| \( N \) | \( g \) | \( \text{rms}(\mathcal{X}_{\alpha,\beta}) \) | \( \text{rms}(M_{\alpha,\beta}) \) | \( \text{rms}(s_N) \) |
|---|---|---|---|---|
| 200 | 3.8 | 0.051\( \Delta \) | 0.031\( \Delta \) | 0.313\( \Delta \) |
| 500 | 6.1 | 0.041\( \Delta \) | 0.020\( \Delta \) | 0.308\( \Delta \) |
| 1000 | 8.6 | 0.034\( \Delta \) | 0.015\( \Delta \) | 0.305\( \Delta \) |

TABLE I: Comparison of the \( 1 / \sqrt{g} \) corrections for different number of electrons, \( N \). We use the relation \( g \approx 0.27 \sqrt{N} \), which is valid for a disc geometry.
of the PSD. As expected, the additional corrections increase the r.m.s. of the spacing with respect to its value in the CEI model (0.28Δ) (see Table I). Notice that 1/√g corrections mainly affect the odd distribution—the even distribution remains essentially unaltered. This is evident in the comparison between the N = 200 and N = 1000 cases (see bottom panel in Fig I). Therefore, both the scrambling and the gate effect are the dominant effects as they are the ones that most affect the δ-function—the effect of the diagonal terms on the δ-function is higher order in 1/g (see discussion in Section III B).

It is important to emphasize that besides the smearing caused by the additional corrections, there is still a noticeable even/odd effect. This theory then does indeed predict such an effect at low T. To what extent this is valid at higher T is discussed next.

VII. TEMPERATURE EFFECTS

So far we have ignored thermal excitations and calculated the PSD in terms of GS energies (Fig I). This will remain a good approximation so long as k_BT ≪ δ, where δ is the energy difference between the GS and the first excited state. In that case, the contribution from the excited states can be ignored. This has been an implicit assumption in most previous work (note however Refs. 16 and 35). We will show now that in the CI model the probability for that to occur is small due to the even/odd effect. This theory then does predict such an effect at low T, to what extent this is valid at higher T is discussed next.

A. GENERAL APPROACH

We now proceed with a detailed calculation. Let us consider the regime Γ ≪ k_BT, Δ ≪ E_C, where Γ is the total width of a level in the QD. Near the CB peak corresponding to the N − 1 → N transition, the linear conductance is given by

\[
G(N) = \frac{e^2}{2k_BT} P_N \sum_{\alpha} \frac{\Gamma_{\alpha}^{L(R)}}{\Gamma_{\alpha}^{L} + \Gamma_{\alpha}^{R}} w_{\alpha}
\]

(42)

with Γα^{L(R)} the partial width of the single-particle level α due to tunneling to the left (right) lead and w_{\alpha} a weight factor given by

\[
w_{\alpha} = \sum_{i,j,\sigma} F_{eq}(j|N) \langle \Psi_j^{N}\rangle \langle e_{\alpha,\sigma}^{\dagger} | \Psi_{i}^{N-1}\rangle^2 (1 - f(\epsilon_j - \epsilon_i)).
\]

(43)

Here, \( P_N^{eq} \) is the equilibrium probability that the QD contains N electrons, \( \hat{H}_{\text{QD}} | \Psi_j^{N}\rangle = \epsilon_j | \Psi_j^{N}\rangle \) so that “j” labels the many-body states of the QD, \( F_{eq}(j|N) \) is the conditional probability that the eigenstate j is occupied given that the QD contains N electrons, and \( f(\epsilon) = \{ 1 + \exp[(\epsilon - E_F)/k_BT]\}^{-1} \). Since near the peak only the states with N − 1 and N electrons are relevant, we have

\[
P_{eq}^N \approx \frac{\exp(-\Omega_N)}{\exp(-\Omega_N) + \exp(-\Omega_{N-1})}
\]

(44)

with \( \Omega_N \) the grand-canonical potential and \( F_N \) the canonical free energy of the QD. To make the dependence on N explicit, let us denote by \{E_j\} the eigenenergies of \( \hat{H}_{\text{QD}} \) without the charging energy term and define \( \delta' = (N - \frac{1}{2}) - N \). Then, \( \epsilon_j - \epsilon_i = E_j^N - E_i^{N-1} + 2E_C\delta'N \) and

\[
F_N - F_{N-1} = -k_BT \ln \left[ \frac{Z_N}{Z_{N-1}} \right]
\]

\[
= E_j^N - E_i^{N-1} + k_BT \ln \left[ \frac{F_{eq}(j|N)}{F_{eq}(i|N-1)} \right] + 2E_C\delta'N
\]

(45)

with \( Z_N \) the canonical partition function. Note that Eq. (45) is valid for any i and j. The contribution of the transition \( i \to j \) to the conductance reaches its maximum when \( f(F_N - F_{N-1})[1 - f(\epsilon_j - \epsilon_i)] \) peaks, namely when

\[
E_F = E_j^N - E_i^{N-1} + \frac{k_BT}{2} \ln \left[ \frac{F_{eq}(j|N)}{F_{eq}(i|N-1)} \right] + 2E_C\delta'N.
\]

(46)

B. Ground state dominated transitions

In the particular case where the transition between GS dominates, and taking the spin degeneracy into account, the CB peak position is given by

\[
E_F = E_{GS}^{N} - E_{GS}^{N-1} - \frac{k_BT}{2} \ln \left[ \frac{2S_{GS}^{N}+1}{2S_{GS}^{N-1}+1} \right] + 2E_C\delta'.
\]

(47)

We see that the peak is shifted with respect to its position at \( T = 0 \) by an amount depending on the change of the spin of the QD. Except for a factor \( \frac{1}{2} \) in front of the entropic term, Eq. (47) corresponds to replacing \( E_{GS}^{N} \) by \( F_N \) in the usual condition for the peak position, which is what we would naively expect at finite temperature. Because the r.m.s. of the PSD is \(~0.3\Delta\) (see Fig. I), this shift is significant even for \( k_BT \sim 0.1\Delta \) and cannot be neglected. Notice that we have not made any assumptions about the Hamiltonian of the QD so far—except that close to the conductance peak it depends...
on the gate voltage only through the charging term. While in the CI model this introduces only a constant shift between the even and odd distributions in the CEI model it changes the shape of both distributions since different spin transitions contribute to each one. Also, one should note that this entropic effect shifts the energy $E_{GS}^N$ in the same direction as the exchange interaction. Then, we should expect an effect on the PSD similar to the one corresponding to an effective increase of $J_S$.

C. Peak conductance

It is important to point out that the magnitude of the on-peak conductance is renormalized because of the spin degeneracy. The reason is that $F_{eq}(j|N)$, the overlap $|\langle \Psi_j^N | e^I_{\alpha,\sigma} | \Psi_j^{N-1} \rangle|^2$ and the value of $P_{eq}^N \times |1 - f(\epsilon_j - \epsilon_i)|$ at its maximum depend on the particular spin transition involved. In the simplest case when only the GS is relevant, we get

$$F_{eq}(j|N) \{ P_{eq}^N |1 - f(\epsilon_j - \epsilon_i)| \} \}_{\text{max}} = \frac{1}{(\sqrt{2S' + 1} + \sqrt{2S + 1})^2}$$

(48)

and

$$\sum_{S'_i, k': S_i, k, \sigma} \left| \langle \Psi_{S'_i, k'} | e^I_{\alpha,\sigma} | \Psi_{S_i, k} \rangle \right|^2 = \begin{cases} 2S' + 1 & \text{if } n_\alpha = 0 \\ 2S + 1 & \text{if } n_\alpha = 1 \end{cases}$$

(49)

where $S'$ ($S$), $S'_i$ ($S_i$) and $k'$ ($k$) are the quantum numbers associated to the state with $N$ ($N-1$) particles. At low temperature, most transitions correspond to the first case in Eq. (49) when $S' > S$ and to the second when $S' < S$. Using that, we finally get

$$G_{\text{peak}} = \lambda \frac{2e^2}{\hbar k_BT} \frac{\Gamma_L^{\alpha} \Gamma_R^{\alpha}}{\Gamma_{\alpha}^{L} + \Gamma_{\alpha}^{R}}$$

(50)

with

$$\lambda = \frac{2(S' + S) + 3}{4 \left( \sqrt{2S' + 1} + \sqrt{2S + 1} \right)^2}$$

(51)

Then, the average conductance peak depends not only on the average coupling to the leads but also on the probability of the transition $S \rightarrow S'$. It is relevant for a quantitative understanding of the low-temperature behavior of $\tilde{\alpha} = 1 - \langle G_{\text{peak}} \rangle_{\text{GOE}} / \langle G_{\text{peak}} \rangle_{\text{GUE}}$ in closed QDs. At $T = 0$, since higher spin is more likely in the GOE case and since $\lambda$ is smaller the bigger the spins involved, this renormalization leads to values of $\tilde{\alpha}$ larger than 0.25—and much larger, of course, depends on $J_S$. At finite temperature, when several transitions contribute to the conductance, it might also lead to values larger than 0.25 and could explain the small deviation observed at low temperature ($k_BT \lesssim 0.4\Delta$) in Ref. [51]. Notice that either the CI model or dephasing processes lead to values smaller than 0.25.

D. Several state case

As we mentioned above, in the general case more than one transition contributes to the conductance, and the CB peak position must be determined by maximizing Eq. (42) with respect to $N$. For arbitrary $T$, this requires the calculation of all possible transitions between the eigenstates of $H_{QD}$ with $N-1$ and $N$ electrons. For simplicity, we restrict ourselves to low enough temperature so that only a few excited states are relevant. Therefore, we kept 6 states in the even case and 4 in the odd one. We checked numerically that at $k_BT = 0.3\Delta$ and for $J_S = 0.28\Delta$, the occupation of these states is, on average, 99.4% (98.3%) for $N$ even (odd), being smaller than 98% (92%) only about 1% of the time. In any case, the effect of temperature can only be underestimated since, in general, different transition leads to different spacing which in turns leads to a smearing of the PSD. Figure 3 shows some of the energy states considered in the calculation of the PSD. For $N$ even, the lowest states with $S = 0$ and $S = 1$ are the dominant states with an occupation of 52.4% and 39.6% respectively at $k_BT = 0.3\Delta$ and $J_S = 0.28\Delta$. In the odd case, those are the lowest states with $S = \frac{1}{2}$ and $S = \frac{3}{2}$, with 80% and 7.5% respectively.

The upper panel in Fig. 3 shows the CEI model PSD for non-zero temperature. Besides the expected smearing of the sharp features and their shift due to the entropic term in $\langle G_{\text{peak}} \rangle_{\text{GUE}}$, there are two important new effects: (a) Temperature alone is able to completely wash-out the $\delta$-function, making the odd distribution broader. Note in addition the long tail for large spacings; we show below that the latter is not simply thermal broadening. (b) The even distribution develops a peak at small spacings—in particular, the maximum of the total distribution is dominated by the even distribution, in sharp contrast to what occurs at $T = 0$. This strongly reduces the relative weight of the long tail in the even case, and the distribution becomes less asymmetric. Actually, the long tail is only slightly affected by...
temperature as it corresponds to large values of the single-particle spacing.

The peak in the even distribution arises from cases where \( S = 1 \) and \( S = 0 \) states are (almost) degenerate. It corresponds to the sharp discontinuity at the origin in the \( T = 0 \) PSD—where both spin states significantly contribute to the conductance. Then, all the transitions with \( \Delta \varepsilon_1 \simeq 2J_S \) collapse into a single (average) value for the spacing, which leads to a peak in the PSD. According to Eq. (46), the corresponding CB peaks are shifted by \( \sim \frac{1}{2} k_B T \ln(4/2) \), which gives a total shift of \( k_B T \ln 2 \) for the peak in the PSD.

Note that the r.m.s. of the distribution is reduced by temperature. In fact, we found that it decreases monotonically from \( T = 0 \).

The fact that more than one transition contributes to the conductance implies that the peak position also depends on the relative strength of the coupling to the leads of the different levels (\( \Gamma_\alpha \)). This should be particularly important when the GS and the first excited state are almost degenerate. The bottom panel of Fig. 3 shows the PSD assuming \( \Gamma_\alpha \equiv \text{cte} \), and using the same parameters as before. It is evident that much of the broadening observed in the top panel is not directly caused by temperature but by the fluctuation of \( \Gamma_\alpha \).

One of the most important differences is the absence of the long tail for large spacing in the odd distribution. This can be easily understood as follows. First, let us note that the sharp jump in the \( T = 0 \) PSD at \( J_S \) results from the transitions involving \( S = \frac{1}{2} \): \( 0 \leftarrow \frac{1}{2} \rightarrow 0, 0 \leftarrow \frac{1}{2} \rightarrow 1, 1 \leftarrow \frac{1}{2} \rightarrow 0 \) and \( 1 \leftarrow \frac{1}{2} \rightarrow 1 \). The spacing in each case is \( J_S, \Delta \varepsilon_2 - J_S, \Delta \varepsilon_1 - J_S \) and \( \Delta \varepsilon_1 + \Delta \varepsilon_2 - 3J_S \), respectively. It is easy to show that at \( T = 0 \), the conditions on \( \Delta \varepsilon_1 \) and \( \Delta \varepsilon_2 \) for each transition to occur, that is for the GS to have the appropriate spin, leads to a spacing \( \leq J_S \) in all the cases. This result is a consequence of the “yes-no” conditions required at \( T = 0 \). At \( T \neq 0 \), those conditions are relaxed and the last three transitions can lead to a spacing bigger than \( J_S \). This thermal broadening is responsible of the disappearance of the \( \delta \)-function. However, because the realizations contributing to that part of the distribution have \( \Delta \varepsilon_1 \simeq 2J_S \), the thermal factors of the different transitions are very similar to each other. Consequently, the relative strength of the couplings can overcome them: the peak position is dominated by the most strongly coupled level, which might correspond to the larger spacing. This explains the larger tail observed when the fluctuation of \( \Gamma_\alpha \) is taken into account.

Similarly, the width of the peak of the even distribution is strongly affected. This clearly indicates that fluctuations of the wavefunctions of the QD strongly modify the PSD.

So far we have discussed temperature effects in the context of the CEI model. It is surprising that, even at this level of approximation, only a weak even/odd effect or asymmetry is expected for \( k_B T \gtrsim 0.3 \Delta \).

E. Corrections to CEI model

Results including the leading order corrections are shown in Fig. 3 for \( k_B T = 0.1 \Delta \) and \( 0.3 \Delta \) with the same parameters as in Fig. 1. The additional fluctuations increase the broadening of the distribution. At low temperature, the effects of the residual interactions are dominant—though the \( T \)-induced peak in the even distribution is evident. For \( k_B T = 0.3 \Delta \), however, temperature is the main effect (compare with Fig. 3). In this case, the even/odd effect is weaker but still noticeable—it should be kept in mind that the experimental noise may contribute significantly to weaken this effect. Also, notice that the PSD is not Gaussian. A detailed analysis of the experimental data of Ref. [5] shows that this is indeed the case. In fact, the agreement between these data and the PSD shown in the lower panel of Fig. 3 is good, both qualitatively and quantitatively.
FIG. 4: Finite temperature CB peak spacing distribution corresponding to the Hamiltonian Eq. (41) with \( J_s = 0.28\Delta, N = 500, \) and \( \delta_{00} = 0.01. \) The top (bottom) panel corresponds to \( k_B T = 0.1\Delta \) (0.3\( \Delta \)) and the solid (dashed) line to \( N \) odd (even).

### VIII. CONCLUSIONS

In this work we have calculated the Coulomb blockade peak spacing distribution including the most representative leading order corrections (up to \( \Delta/\sqrt{3} \)) to the CEI model as well as the effect of finite temperature.

At \( T = 0 \), our results show that the PSD still presents a clear signature of an even/odd effect. Even though it is much weaker than the effect predicted by the CI model, it is definitely big enough to be observable. No sharp features remain, and the peak in the odd distribution (the former \( \delta \)-function) is still the dominant characteristic. Also, the distribution is far from being Gaussian and its width is \( \sim 0.3\Delta \). This number, however, depends on the value of \( J_S \) and on many geometry-dependent parameters that could vary a bit for the actual QD. On the other hand, it could be argued that the RPA approach used in the calculation of the screening of the Coulomb potential is not appropriate for \( r_s \sim 1 \). We think, however, that the essential ingredients are captured by this approach and that any correction that would arise from a more accurate calculation could be included by a renormalization of \( E_C \) and \( J_S \). Such a renormalization could have an important impact both in the shape of the distribution and in the strength of even/odd effect since they are quite sensitive to the value of \( J_S \). An experimental determination of \( J_S \) should, then, be a high priority.

For \( T \neq 0 \) the picture is quite different. At \( k_B T \sim 0.3\Delta \), the roles of the even and odd distribution are inverted: it is the even distribution that shows a peak, while in the odd one the \( \delta \)-function is washed-out. This is very important, since the absence of the \( \delta \)-function has been one of the puzzles in interpreting the experimental results. The final distribution is closer to a Gaussian-like shape, and the even/odd effect is much weaker. Here, the main effect in the distribution comes from the temperature. One important consequence of the finite temperature is that the fluctuation of the coupling to the leads becomes relevant and substantially contributes to the broadening of the PSD. Both the shape and the r.m.s. of the distribution agree with the data in Ref. \( 15 \). We should mention however, that we fail in reproducing the long tail for small spacing. This could be due to (a) relevance of higher excited states—note that this part of the distribution corresponds to cases where the single-electron spacing is very small—and the consequent effect of the fluctuation of the couplings, or (b) mixing of the top levels caused by the off-diagonal terms of the interaction—here our second order perturbation theory fails—or by the off-diagonal terms of the scrambling. At lower \( T \) both distributions show a peak, which is a clear observable feature.

It is important to point out that our results do not explain the data of either Ref. \( 17 \) or \( 18 \). Nevertheless, in both cases there are some elements to think that this is not a “failure” of the model. In Ref. \( 17 \) the interpretation of the transport process itself is not clear. For example, the width of the CB peak is not controlled by temperature though its shape corresponds to a thermally assisted process. In Ref. \( 18 \) temperature effects are negligible due to both \( k_B T \sim 0.05\Delta \) and \( J_S \sim 0.25\Delta \). However, the single-particle dynamics is not fully chaotic because of the regular shape of the QD. Therefore, the effect of regular orbits and of the presence of regular islands in phase space, must be considered. This could enhance the contribution of \( \Pi_B \) in Eqs. (11) and (12) and lead to larger fluctuations of both \( M_{\alpha,\beta} \) and \( A_{\alpha,\beta} \). This subject is quite complex and we leave it for future work. Nevertheless it is important to mention that the r.m.s. in Ref. \( 18 \) is of order \( 0.4\Delta \) and that there is a weak even/odd effect.

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APPENDIX A: THE DIFFUSIVE CASE

Similar results for the leading order corrections can be obtained in the case of diffusive QDs after the appropriate change of some definitions. First, the dimensionless conductance is now given by \( g = \hbar \gamma_1 / \Delta \) where \( \gamma_1 \) is the smallest non-zero eigenvalue of the diffusion equation, \(-D\nabla^2 f_n(r) = \gamma_n f_n(r)\), supplemented with von Neumann boundary conditions. \( D = v_p \ell / 2 \) is the diffusion constant and \( \ell \) the mean free path. Second, \( k(r_1, r_2) = \exp(-r/\ell) J_0^2(kr) \) with \( r = |r_1 - r_2| \). Third, the propagator \( \Pi_B(r_1, r_2) \) is replaced by its diffusive counterpart

\[
\Pi_B(r_1, r_2) = \frac{\Delta A}{\pi} \sum_n \frac{f_n(r_1) f_n(r_2)}{\hbar \gamma_n}.
\]

(A1)

In order to obtain a numerical value for the fluctuation of the different matrix elements, a specific geometry must be assumed. For a disc of radius \( R \) we get,

\[
\gamma_{m,n} = \frac{D \beta_{m,n}^2}{R^2}, \quad J_m'(\beta_{m,n}) = 0
\]

(A2)

and

\[
f_{m,n}(r) = A_{m,n} \left\{ \cos m\phi \left\{ J_m^2(\beta_{m,n} r/R) \right. \right\}
\]

(A3)

with

\[
A_{m,n} = \sqrt{\frac{2}{(1+\delta_{m,0})\pi R \sqrt{\beta_{m,n}^2 - m^2}}} J_m(\beta_{m,n})
\]

(A4)

Here, \( J_m(x) \) is a Bessel function and \( J_m'(x) \) its derivative. Note that the first non-zero eigenvalue, \( \gamma_{1,1} \), is proportional to the square of the first zero of \( J_1' \), \( \beta_{1,1} \approx 1.84 \). This means that the last mode to relax is the one with the smallest number of nodes in the angular direction and none in the radial direction (except for the origin), \( J_{1,1}(r) \propto \cos \phi J_1^2(\beta_{1,1} r/R) \). Then, \( g = \hbar D \beta_{1,1}^2 / R^2 \Delta \propto \ell / R \sqrt{N} \). For \( N \sim 500 \) and \( \ell \sim R/2 \) this gives \( g \approx 13 \).

1. Scrambling

The main contribution in this case comes from the second term in Eq. \( \text{(14)} \). Because there is no reason to assume a \( 1/r \) decay of the wavefunction correlation in a general case, we cannot use the same approach we used in Section \( \text{V} \). Instead, we assume a disc geometry to get

\[
b_{00} = \frac{1}{\pi A} \sum_{\gamma_{0,n} > 0} \frac{\gamma_{1,1}}{\gamma_{0,n}} \left[ \int dr V(r) f_{0,n}(r) \right]^2
\]

\[
= \frac{1}{4\pi} \sum_{\beta_{0,n} > 0} \frac{\beta_{1,1}^2}{\beta_{0,n}^4} \sin^2(\beta_{0,n}) J_0^2(\beta_{0,n})
\]

(A5)

which is very close to the value obtained for the ballistic case. Here we used \( V(r) = 1/4[1 - (r/R)^2] \). Thus \( \text{var}(X_{\alpha,\beta}) \) remains of the same order as in the ballistic case.

2. Diagonal elements

In this case, the terms in Eq. \( \text{(13)} \) that involve \( k(r_1 - r_2) \) are small (assuming \( \ell \ll \sqrt{A} \)) and can be neglected. Then

\[
\text{var}(M_{\alpha,\beta}) = \frac{\Delta^2}{4A^2} \int \text{d}r_1 \text{d}r_2 \left| \Pi_D(r_1, r_2) \right|^2.
\]

(A6)

Assuming a disc geometry we get

\[
\text{var}(M_{\alpha,\beta}) = c_2 \Delta^2 / 4g^2
\]

with

\[
c_2 = \frac{1}{\pi^2} \sum_{\gamma_{m,n}} \left( \frac{\gamma_{1,1}}{\gamma_{m,n}} \right)^2
\]

(A7)

\[
= \frac{2}{\pi^2} \sum_{m=0}^{\infty} \sum_{n=1}^{\infty} \left( \frac{\beta_{1,1}}{\beta_{m,n}} \right)^4
\]

\[
\approx 0.13
\]

Once again, the numerical result is similar to the one we obtained for the ballistic case. For instance, using \( N \sim 500 \) and \( \ell \sim R/2 \), we get \( \text{var}(M_{\alpha,\beta}) \approx 0.014 \Delta \), which should be compared with the second row in Table \( \text{I} \).

APPENDIX B: SECOND ORDER CORRECTION FOR \( S = \frac{1}{2} \)

We give here an explicit expression for the second order correction to the energy due to the off-diagonal terms for the case of \( S = \frac{1}{2} \).
\[ E^{(2)}_{S=\frac{1}{2}} = \sum_{\beta \geq \alpha, \gamma \geq \delta} \frac{3|a_{\alpha,\beta,\gamma,\delta}|^2 + |a_{\alpha,\beta,\gamma,\delta}|^2}{\varepsilon_{\alpha} + \varepsilon_{\beta} - \varepsilon_{\gamma} - \varepsilon_{\delta}} (1 - \frac{\delta_{\alpha,\beta}}{2}) (1 - \frac{\delta_{\gamma,\delta}}{2}) + \sum_{\alpha, \gamma \geq \delta} \frac{3|a_{\alpha,1,\gamma,\delta}|^2 + |a_{\alpha,1,\gamma,\delta}|^2}{2(\varepsilon_{\alpha} + \varepsilon_{1} - \varepsilon_{\gamma} - \varepsilon_{\delta})} (1 - \frac{\delta_{\gamma,\delta}}{2}) + \sum_{\beta, \gamma} \frac{3|a_{\alpha,\beta,1,\alpha,1,\gamma}|^2 + |a_{\alpha,\beta,1,\alpha,1,\gamma}|^2}{2(\varepsilon_{\beta} - \varepsilon_{\gamma})} + \sum_{\gamma} \frac{|a_{\alpha,1,\gamma,\alpha}|^2}{4(\varepsilon_{\beta} - \varepsilon_{\gamma})} \]  

(B1)

where \( \alpha \) and \( \beta \) (\( \gamma \) and \( \delta \)) correspond to doubly occupied (empty) levels of the \( S = \frac{1}{2} \) state—except for the term with \( \sum \) in which case the singly occupied level labeled “1” is included. Note that there are several terms which add coherently.
Note that in the case of a diffusive QD, this term gives the main contribution to the variance (see Appendix A), which turns out to be of the same order as the first term in the ballistic case. It might also be important in systems with strong semiclassical effects.

One should note, however, that the covariance between the matrix elements $M_{\alpha,\beta}$ and $M_{\gamma,\beta}$ is of order $\Delta^2/g^3$ (see Ref. 57 for details) which, in general, also leads to a correction of order $\Delta/\sqrt{g}$ to the spacing. For a diffusive QD, this term is small due to the exponential decay of $k(r_1-r_2)$, but it might be important in cases with strong semiclassical effects.

With this definition, $s_N$ has the classical result $2E_C$ subtracted. That is, $s_N = 0$ ($\Delta \varepsilon$) for the odd (even) case in the CI model.

This is no longer true once the gate effect is introduced. However, taking this into account would introduce a correction of order $\Delta/E_C \times \text{rms}(X_{\alpha,\beta})$, which is negligible.

The quantum numbers $S$ and $S_z$ are not enough to specify a many-body state if the number of singly occupied levels is bigger than 2, even for a given set $\{n_\alpha\}$ of occupation numbers (see Ref. 43).

Notice, however, that $\tilde{\alpha}$ always first decreases from its $T = 0$ value and then increases again. This is related to the fact that the contribution from the excited states come first in the GOE case.

Because the fluctuations of the single particle levels, this is of course always violated for some (very) rare realizations. This prevents us from describing the asymptotic regime on the left side of the PSD in Fig. 3 and 4.