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 predicts 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: (i) its peak is dominated by the even distribution at $k_BT \sim 0.3\Delta$ (at lower $T$ a double peak appears), (ii) the even/odd effect is considerably weaker, (iii) the $\delta$ function is completely washed out, and (v) fluctuation of the coupling to the leads becomes relevant. Experiments aimed at observing the $T=0$ peak spacing distribution should therefore be done at $k_BT<0.1\Delta$ for typical values of the e-e interaction.

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I. INTRODUCTION

The Coulomb blockade (CB) of electron tunneling is one of the most studied effects in quantum dots (QDs).1–6 It allows one to probe quantum interference effects in both the wave function 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 the end reasonable quantitative agreement between theory and experiment is obtained.

The CB effect occurs when the thermal energy $k_BT$ is smaller than the charging energy $E_C = e^2/2C$ required to add an electron to the QD—$C$ is the total capacitance of the QD. In that case, electron transport through the QD is blocked by energetics, fixing the number of electrons $N$ in the QD. By sweeping the voltage $V_g$ of a capacitively coupled gate, this CB can be overcome at a particular value $V_g^N$, where the transition $N\to N+1$ occurs. The conductance $G(V_g)$ shows then a series of sharp peaks as a function of $V_g$ as additional electrons are added to the QD. At sufficiently low temperature, only the ground state (GS) contributes significantly to the conductance peak. The position of the CB peak is then proportional to the change in the GS energy of the QD upon adding one electron.4

The simplest model used for the description of this phenomenon assumes a constant e-e interaction—hence the name constant interaction (CI) model. The single-particle part of the Hamiltonian is described by random matrix theory (RMT) under the assumption that the single-particle classical dynamics is chaotic (or diffusive). As a result, the fluctuation of both the conductance peak height and the CB peak spacing is given by single-particle RMT statistics. Despite the success of this model in explaining the former7—once thermal8,9 and periodic orbit effects10–12 are included—it fails drastically in describing the observed PSD.13–18

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 has shown such an effect—though a weak even/odd effect was observed18,19—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 experiments13,14 found it scaled with $E_C$, which is much bigger than the predicted value, $\Delta$, the single-particle mean level spacing. More recent experiments,15,17,18 however, showed that it is indeed of order $\Delta$.

The search for an explanation for these discrepancies triggered several theoretical works over the last years.13,20–31 Fueled by the earlier experiments,13,14 it was suggested13,20,22,23 that GS fluctuations were dominated by the e-e interaction itself. Therefore, a completely different approach—invoking nonperturbative 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, $N \gg 1$,32 it was argued21,24–31,33 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 experimental data.\textsuperscript{15,19}

The small parameter in this perturbative approach is $1/g$ with $g = E_{\text{th}}/\Delta$ the dimensionless conductance and $E_{\text{th}}$ the Thouless energy (approximately $\hbar$ times the inverse time of flight). The condition for the QD to be a good conductor is $g \approx \sqrt{N} \gg 1$.\textsuperscript{5,31} Interaction corrections are classified by their order in $1/g$ 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.\textsuperscript{25–27,29} 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, such as the CB peak spacing, that are sensitive to single levels in the QD. The zero-order Hamiltonian---hereafter the constant exchange and interaction (CEI) model---is given by\textsuperscript{6,27,31}

$$H_{\text{CEI}} = \sum_{a,\alpha} \varepsilon_a \hat{n}_{a,\alpha} + E_{\text{C}}(\hat{n} - N)^2 - J_S \hat{S}^2,$$

where $\{\varepsilon_a\}$ are the self-consistent single-electron energies in the mean-field potential,\textsuperscript{29,34} $N = C_g V / e$ describes the capacitive coupling to the control gate, $C_g$ is the dot-gate capacitance, $\hat{S}$ 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 $\hat{S}^2$. Because it sometimes leads to a GS with $\hat{S} = 1$, the simple “up-down” filling scheme breaks down.\textsuperscript{20,21,25–27,35} The corresponding PSD is completely different from the CI model result (see Ref. 29 for a plot). In fact, a GS with $\hat{S} = 1$ has been experimentally observed very recently.\textsuperscript{30} 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 (i) the “scrambling” of the spectrum when adding an electron to the QD,\textsuperscript{21} (ii) the fluctuation of the diagonal matrix element of the $e$-$e$ interaction,\textsuperscript{29} and finally, not related to the $e$-$e$ interaction, (iii) the change in the single-electron energies when the gate voltage is swept.\textsuperscript{24} 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.\textsuperscript{24,37} We also show that the fluctuation of the off-diagonal matrix elements\textsuperscript{28,38} 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,\textsuperscript{30} we pointed out that there is a simple effect that has not been taken into account: finite temperature---we should mention though that temperature effects have been discussed previously for spinless particles.\textsuperscript{16,37} In our previous paper,\textsuperscript{30} we show 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. 18---our results are crucial for interpreting the experimental data. Here, we present details of those results and extend them to the experimental range. 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 Sec. II we briefly review the arguments that lead to the CEI model. The leading-order corrections to this model are introduced in Sec. III. We calculate the contribution of the off-diagonal terms of the $e$-$e$ interaction and the magnitude of the scrambling effect in Secs. IV and V, respectively. Numerical results for the $T = 0$ PSD, including all the corrections, are presented in Sec. VI. We introduce the effect of finite temperature in Sec. VII. Finally, we conclude in Sec. VIII.

\section{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) QD’s, 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 $E_{\text{th}}$. 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’s (see Refs. 5 and 39 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 $E_{\text{th}}$. 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 (RPA). In that case, the screened potential reads\textsuperscript{5,21}

$$V_{\text{sc}}(r_1, r_2) = \frac{e^2}{C} + V_{\text{TF}}(r_1, r_2) + V(r_1) \Delta + V(r_2) \Delta,$$

where $C$ is the capacitance of the QD, $V_{\text{TF}}(r)$ 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 Sec. V. Here and throughout this paper we consider two-dimensional (2D) quantum dots. The last three terms in Eq.
are of order $\Delta$ and thus much smaller than the first term. This leads to the following Coulomb interaction Hamiltonian

$$\hat{H}_{\text{int}} = E_C n^2 - \hat{n} + \hat{\mathcal{H}}_{\text{int}}.$$  

where

$$\mathcal{H}_{\alpha,\beta} = \frac{1}{2} \sum_{a,b} H_{\alpha,\beta} \delta_{a,b} \mathcal{C}_{\alpha,\beta}^\dagger \mathcal{C}_{\alpha,\beta},$$

(3)

and

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

(5)

where $J' = A^{-1} \int \mathcal{V}_T \mathcal{V}_T (r_1 - r_2) \mathcal{V}_T (r_1 - r_2)$ is a classical propagator. 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 $\mathcal{H}_{\text{QD}}$, which only takes the universal part of the residual interactions into account. Here, we include the next-order corrections: (i) the “scrambling” of the spectrum when adding an electron to the QD; (ii) the fluctuation of the diagonal part of the $e-e$ interaction; (iii) the change in the singlet–singlet energies when the gate voltage is swept. Although (ii) is a correction of order $\Delta/g$ to the Hamiltonian, all three effects lead to corrections of order $\Delta/\sqrt{g}$ to the spacing. We now discuss each of them in detail.

#### A. Scrambling

The scrambling effect is caused by the presence of the potential $\mathcal{V}(r) \Delta$ in Eq. (2), which leads to the second term in Eq. (3). 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, $\mathcal{V}(r) \Delta$, for the electrons inside the QD. While in 3D materials the charge is confined to a small region near the surface, in two dimensions it is inhomogeneously distributed over the whole area of the QD.

It is straightforward to show that $\langle X_{\alpha,\beta} \rangle = \mathcal{V} \Delta \delta_{\alpha,\beta}$ where

$$\mathcal{V} = A^{-1} \int \mathcal{V}_T \mathcal{V}_T (r).$$

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 $X_{\alpha,\beta}$. In particular, the main contribution (to the spacing) arises from $X_{\alpha,\alpha}$, with $\alpha$ the top level. Its variance is given by

$$\text{var}(X_{\alpha,\alpha}) = \Delta^2 \int \mathcal{V}_T \mathcal{V}_T (r_1) \mathcal{V}_T (r_2) \langle |\Psi_{\alpha}^\dagger (r_1) \Psi_{\alpha} (r_2)|^2 \rangle$$

(9)

with $\mathcal{V}(r) = \mathcal{V}(r) - \mathcal{V}$. With corrections of order $1/g$ included, the wave-function correlation appearing in Eq. (9) is given by

$$A^2 \langle |\Psi_{\alpha}^\dagger (r_1) \Psi_{\alpha} (r_2)|^2 \rangle = 1 + k(r_1, r_2) - k(r_1) - k(r_2) + k$$

(10)

with $k(r_1, r_2) = J_0^2 (k_1 r_1 - r_2)$, $k(r) = A^{-1} \int \mathcal{V}_T \mathcal{V}_T (r)$, and

$$\Pi_B (r_1, r_2)$$

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 $\int d\mathbf{r}_1 \Pi_B(r_1,r_2) = 0$ 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 wave functions is given by a random superposition of plane waves.\textsuperscript{46} The other terms involving $k(r_1,r_2)$ properly account for the normalization of the wave functions.\textsuperscript{45}

For quantitative evaluation we consider the case of a ballistic circular disc with diffusive boundary conditions. For this system,\textsuperscript{44} the term involving $\Pi_B(r_1,r_2)$ yields 0 exactly since the potential $V(r)$ is isotropic (in the isolated dot case, see Sec. 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($\lambda_{a,a}$) is correct up to a factor $2^4$.\textsuperscript{47}

Since $k(r_1,r_2) = 1/\pi k_F |r_1-r_2|$, a simple dimensional analysis shows that Eq. (9) is proportional to $\Delta^2/k_F \sqrt{A}$ so that\textsuperscript{6,21}

$$\text{var}(\lambda_{a,a}) = b_{00} \frac{\Delta^2}{g}. \quad (11)$$

The same result is valid for var($\lambda_{a,b}$). Again using the circular disc with diffusive boundaries for quantitative estimation, we have $E_0 = h \gamma V_F / R$ so that $g = \gamma_1 k_F \sqrt{A} / 2\pi$ with $\gamma_1 = 0.38^6,21,44$ The approximate value of the geometry-dependent coefficient $b_{00}$ is calculated in Sec. V.

**B. Diagonal matrix elements**

Fluctuation of the diagonal terms of $\hat{H}_{\text{int}}$ leads to a correction to the spacing of the same order as the scrambling.\textsuperscript{29} In the zero-range approximation, where the short-range screened potential is approximated by a $\delta$ function, $V_{TF}(r) = \delta(r) \Delta A/2$, the variance of the diagonal elements is given by\textsuperscript{43,48}

$$\text{var}(M_{a,b}) = \frac{\Delta^2}{4A^2} \int d\mathbf{r}_1 d\mathbf{r}_2 \left[ (\vec{k}(r_1-r_2))^2 + 2[\Pi_B(r_1,r_2)]^2 \right]$$

$$+ 4\vec{k}(r_1-r_2)\Pi_B(r_1,r_2), \quad (12)$$

where $M_{a,b} = H_{a,a} - \langle H_{a,a} \rangle$. Using the full expression for $V_{TF}$, the variance of the diagonal elements leads to similar numerical results\textsuperscript{29}—in that case it is important to keep the correlation between the direct and the exchange terms. The dominant contribution in Eq. (12) comes from $|k(r_1-r_2)|^2$—the other terms are of the same order in $1/g$ but numerically much smaller—so

$$\text{var}(M_{a,b}) = \frac{3\Delta^2}{4\pi} \frac{\ln(4k_F \sqrt{A})}{(k_F \sqrt{A})^2} \frac{\ln g}{g^2} \Delta^2. \quad (13)$$

For the double-diagonal matrix element, var($M_{a,a}$) = $4\text{var}(M_{a,b})$.\textsuperscript{29}

Let us now consider the contribution of the fluctuation of the diagonal terms to the spacing corresponding to the transition $\frac{1}{2} \rightarrow 0 \rightarrow \frac{1}{2}$.
see the next section and Ref. 6 for more details. The former is the same potential that appears in Eq. (2) and causes the scrambling 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 nonuniform distribution of charge, which creates $V(r)\Delta$; vice versa, an extra charge must be distributed in the same way so that the potential of the QD is uniform. Equation (16) leads to the following correction to the Hamiltonian:

$$\hat{H}_{\text{gate}} = - \sum_{\alpha,\beta,\sigma} c_{\alpha,\sigma}^\dagger \chi_{\alpha,\beta,\sigma} + \sum_i \delta N_i \chi_i^\dagger \chi_i,$$  

(17)

where $\chi_i^\dagger$ is the matrix element of $V^{(i)}(r)$, in analogy to $\chi_{\alpha,\beta}$ defined above. It is then clear that $\chi_i^\dagger \chi_{\alpha,\beta} = b_i \Delta^2 / g$, with $b_i$ a geometry dependent numerical coefficient.

Notice that the change in the shape of the QD can be associated with the last term in Eq. (16). For instance, if the potentials of two plunger gates are swept in a way such that $\delta N = \delta N_1 + \delta N_2 = 0$ 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.\(^{16}\) Notice that the change in the shape of the QD can be isolated.\(^{16}\) Note, however, that this procedure actually tests only the difference between $V^{(1)}(r)$ and $V^{(2)}(r)$, which could be smaller than 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.\(^{28,38}\) 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),

$$E_S^{(2)} = \sum_j |\langle \Psi_S^N | \hat{H}_{\text{int}}^{\text{off}} | \Psi_S^N \rangle|^2 / E_S^{(0)} - E_j^{(0)},$$  

(18)

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

Following Ref. 38, we rewrite the off-diagonal part of the Hamiltonian in Eq. (3) as follows,

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

(19)

with

$$u_{\alpha,\beta,\gamma,\delta} = H_{\alpha,\beta,\gamma,\delta} - H_{\alpha,\beta,\gamma},$$

$$a_{\alpha,\beta,\gamma,\delta} = H_{\alpha,\beta,\gamma,\delta} - H_{\alpha,\beta,\gamma,\delta}.$$  

(20)

The sum in Eq. (19) runs over all configurations in which the indices of $c_{\gamma}^\dagger$ and $c_{\delta}$ 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.\(^{38}\) 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. (18) 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 $|\Psi_j^N\rangle$. This complication arises because (i) the indices in Eq. (19) might be partially paired, so terms within each of the two main terms do not necessarily produce orthogonal states, or (ii) nontrivial states, such as the $S = 1$ state, can lead to the same final state under the action of any of the two main terms in Eq. (19) for particular values of the indices. In order to avoid the first problem, we explicitly take into account all the possible pairings of the indices and rewrite Eq. (19) as

$$\hat{H}_{\text{int}}^{\text{off}} = \hat{H}_A + \hat{H}_B + \hat{H}_C$$  

(21)

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

\[ \hat{H}_B = \sum_{\alpha, \gamma} \sum_\sigma \left[ a_{\alpha, \gamma, \sigma} c_{\alpha, \sigma} \right] + \sum_{\alpha, \gamma} \sum_\sigma \left[ a_{\alpha, \gamma, \sigma} c_{\alpha, \sigma} + a_{\alpha, \gamma, \sigma} c_{\alpha, \sigma} \right] + \sum_{\alpha, \gamma} \sum_\sigma \left[ a_{\alpha, \gamma, \sigma} c_{\alpha, \sigma} - a_{\alpha, \gamma, \sigma} c_{\alpha, \sigma} \right] \]

\[ \hat{H}_C = \sum_{\alpha, \beta, \gamma} \sum_\sigma \left[ a_{\alpha, \beta, \gamma, \sigma} c_{\alpha, \sigma} + a_{\alpha, \beta, \gamma, \sigma} c_{\alpha, \sigma} \right] \]  

and \( \hat{H}_C \) as in Eq. (19) 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. (19).

In general, the eigenstates of \( \hat{H}_{CEF} \) are a superposition of Hartree-Fock (HF) states. However, because \( S^2 \) and the single-particle Hamiltonian commute, they can be classified by their occupation numbers \( \{ n_a \} \). 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 \( N_s = 3 \), the values of \( S \) and \( S_z \) are not enough to specify a given eigenstate—for 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. (18) for an arbitrary state \( | \Psi_S \rangle \). 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, \( \langle \Psi_S \rangle \) has only doubly occupied levels (up to \( E_F \)). It is easy to see that the last two terms of \( \hat{H}_A \) give zero when applied in \( | \Psi_S \rangle \). The remaining terms of \( \hat{H}_A \) give

\[ \hat{H}_A | \Psi_S \rangle = \sum_{\beta, \gamma} \left[ \begin{array}{c} \sum_\alpha \frac{1}{2} (3 u_{\alpha, \beta, \gamma, a} + a_{\alpha, \beta, \gamma, a}) \\ \frac{1}{2} (3 u_{\alpha, \beta, \gamma, a} + a_{\alpha, \beta, \gamma, a}) \end{array} \right] | \Psi_S \rangle. \]  

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 \( \hat{H}_C \) leads to orthogonal states. Adding up all the contributions, we finally get the following expression,

V. MAGNITUDE OF SCRAMBLING EFFECT

As we mentioned in the previous section, the origin of the potential \( V(r) \) in Eq. (2) 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, $\text{var}(\mathcal{X}_{\alpha,\beta}) = b_{00}\Delta^2/g$, 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 a 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 explain 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. 6 we write

$$V(r) = \frac{A_k}{8\pi C} \int dr_2 \tilde{\partial}_r \tilde{\partial}_z D(r_2, r_2), \quad (26)$$

where $\tilde{\partial}_z = \partial_z - \partial_\gamma$ (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, and

$$C = \left[ \frac{\kappa}{4\pi} \int dr_1 dr_2 \tilde{\partial}_r \tilde{\partial}_z D(r_1, r_2) \right] \quad (27)$$

is the total capacitance of the QD. Equation (26) has a very clear physical interpretation if we notice that

$$\phi(r) = -\frac{e}{C} \int dr_2 \tilde{\partial}_r \tilde{\partial}_z D(r_2, r_2) \quad (28)$$

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

$$V(r) = -\frac{A_k}{2e} \sigma(r) \quad (29)$$

with $\sigma(r)$ the surface charge density on the QD associated with the electrostatic potential $\phi(r)$. Using Eq. (27), it is straightforward to show that $Q = \int d\sigma(r) = -e/C$; note that this implies $V = \tilde{z}$. Introducing Eq. (29) in Eq. (9) and using the fact that $k(r_1, r_2) = \int \frac{dr_1 dr_2}{\pi k_1 k_2}$ we get

$$\text{var}(\mathcal{X}_{\alpha,\beta}) = \frac{\Delta^2}{4\pi k_{\text{eff}}^{3/2}} \left[ \frac{1}{A^{3/2}} \int \frac{dr_1 dr_2}{|r_1 - r_2|} \right.
\left. + \sqrt{\frac{A}{Q^2}} \int dr_1 \sigma(r_1) \frac{2Q}{A} \phi'(r_1) \right], \quad (30)$$

where

$$\phi'(r_1) = \int dr_2 \frac{\sigma(r_2)}{|r_1 - r_2|} \quad (31)$$

is the potential due to the surface charge on the QD. Note that in the presence of close top gate, $\sigma(r) \approx \text{const.}$ and then var$(\mathcal{X}_{\alpha,\beta}) \approx 0$. 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 allows us to readily obtain

$$\text{var}(\mathcal{X}_{\alpha,\beta}) = \frac{\Delta^2}{4\pi k_{\text{eff}}^{3/2}} \left[ \alpha - \frac{\sqrt{A}}{C} \right], \quad (32)$$

with $\alpha = A^{3/2} \int dr_1 dr_2 |r_1 - r_2|^{-1}$. Notice that no particular geometry has been assumed so far. The first term in the parentheses can be calculated numerically for arbitrary geometries. The second, however, requires the calculation of the capacitance. In the case of an ellipsoidal QD, \[ \frac{\sqrt{A}}{C} = \sqrt{\frac{b}{a}} \left\{ \arcsin \frac{1}{\sqrt{x^2 - 1}} \right. \times \sqrt{1 - \left( \frac{b^2}{a^2} \right)^2}, \quad (33) \]

where $a (b)$ is the length of the long (short) axis and $F(\phi, \mu)$ is the elliptic integral of the first kind. For $a/b = 1 - 3$ we get $b_{00} \approx 0.002$. It is clear then that $\text{rms}(\mathcal{X}_{\alpha,\beta}) \approx 0.04\Delta/\sqrt{g}$ 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 37.

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. (32), 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 $\tilde{\phi}' = A^{3/2} \int dr \phi''(r)$ and $\beta = \left( \tilde{Q} \tilde{\phi}' \right)^{-1} \int dr \sigma(r) \phi''(r)$ we find

$$\text{var}(\mathcal{X}_{\alpha,\beta}) = \frac{\Delta^2}{4\pi k_{\text{eff}}^{3/2}} \left[ \alpha - \frac{\sqrt{A}}{C} \right] \left( 1 + (2 - \beta) \frac{\tilde{\phi}'}{e/C} \right), \quad (34)$$

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

Since $\beta \sim 1$ and $\tilde{\phi}'>0$ (the sign of the induced charge is the opposite of $Q$), it is evident that using the isolated dot result [Eq. (32)] gives an upper limit to 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 $\tilde{\phi}'' = \sum_{i} Q_i / d_i \kappa$, with $d_i$ the distance between the centers of charge of the QD and the $i$th gate. Since $Q_i = -C_i d_i (-e/C)$, where $C_i$ is the dot-$i$th gate capacitance, it turns out that $\tilde{\phi}''/(e/C) = \sum_{i} C_i d_i / d_i \kappa$. Then,
where we use that typically $\Sigma_i C_i' / C \sim 0.5$ and denote by $d$ the average distance between the center of the dot and the gates. For the data of Ref. 15 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.24,37

**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

$$s_N = [E_{GS}^{N+1}(\mathcal{N}) - E_{GS}^{N}(\mathcal{N}')] - [E_{GS}^{N}(\mathcal{N}) - E_{GS}^{N-1}(\mathcal{N})],$$

where $E_{GS}^{N}(\mathcal{N})$ is the GS energy of the QD with $N$ electrons excluding the charging energy term and $\mathcal{N}$ is the corresponding gate voltage.24 Including all the leading-order corrections to the CEI model, the Hamiltonian reads

$$\hat{H}_{QD} = \hat{H}_{CEI} + \frac{1}{2} \sum_{a,b,\gamma,\delta} H_{a,b,\gamma,\delta} C_a^\dagger \sigma_a^\dagger C_b \sigma_b + \sum_{a,b,\gamma,\delta} C_a^\dagger \sigma_a^\dagger C_b \sigma_b + \delta N \delta N' \delta N''$$

where the variance of $H_{a,b,\gamma,\delta}$ and $\delta N$ is given by Eq. (13) and Eq. (34), respectively. Their mean values are included in the definition of $E_C$ and $J_S$, so that $\langle H_{a,b,\gamma,\delta} \rangle = \langle \delta N \rangle = 0$. The second term in Eq. (37) includes only the diagonal terms of the residual interaction, and $\delta N$ 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 $N+2$ at the corresponding $\mathcal{N}$, $\mathcal{N}'$, and $\mathcal{N}''$. We only kept two consecutive spacings for each realization of the single-particle Hamiltonian. It is worth mentioning again that Eq. (37) is defined in a window up to $E_{\text{th}}$, so that only $g$ levels were considered.

The parameters we use are (i) $g = 0.38 \sqrt{N/2}$ (which corresponds to a disk geometry),21,23 (ii) the upper limit for the value of $b_{00} \approx 0.01$, and (iii) $b_{11} = b_{00}$. Only transitions with $|\delta S| = \frac{1}{2}$ were taken into account since in the case of spin-orbit interaction (or if it is small), the transitions where the change in the GS spin is bigger than $\frac{1}{2}$, appear as “missing” peaks in the conductance and are not included in the experiment.

Numerical results for $N = 200, 500, 1000$ 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. 29. 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 of the PSD. As expected, the additional corrections increase the rms of the spacing with respect to its value in the CEI model (0.28$\Delta$) (see Table I). Notice that $1/\sqrt{g}$ 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 panels in Fig. 1). Therefore, both the scrambling and the gate effect are the dominant effects as they are the ones that most affect the $\delta$ function—the effect of the diagonal terms on the $\delta$ function is higher order in $1/g$ (see discussion in Sec. 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.

**TABLE I.** Comparison of the $1/\sqrt{g}$ corrections for different numbers of electrons, $N$. We use the relation $g = 0.27 \sqrt{N}$, which is valid for a disk geometry (Ref. 42).

<table>
<thead>
<tr>
<th>$N$</th>
<th>$g$</th>
<th>$\text{rms}(X_{a,b})$</th>
<th>$\text{rms}(M_{a,b})$</th>
<th>$\text{rms}(s_N)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>200</td>
<td>3.8</td>
<td>0.051$\Delta$</td>
<td>0.031$\Delta$</td>
<td>0.313$\Delta$</td>
</tr>
<tr>
<td>500</td>
<td>6.1</td>
<td>0.041$\Delta$</td>
<td>0.020$\Delta$</td>
<td>0.308$\Delta$</td>
</tr>
<tr>
<td>1000</td>
<td>8.6</td>
<td>0.034$\Delta$</td>
<td>0.015$\Delta$</td>
<td>0.305$\Delta$</td>
</tr>
</tbody>
</table>
VII. TEMPERATURE EFFECTS

So far we have ignored thermal excitations and calculated the PSD in terms of GS energies (Fig. 1). This will remain a good approximation so long as \( k_B T \ll \delta \), where \( \delta \) 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 37). We will show now that in the CEI model the condition for achieving \( k_B T \ll \delta \) is much more restrictive than in the CI model and that in fact temperature effects are crucial for understanding the experimental data.\(^{30}\)

There are two simple reasons to expect stronger temperature effects in the presence of exchange. First, there is a change in the occupation of the excited states. For example, assuming \( N \) even, we have \( \delta = |\Delta e - 2J_s| \), with \( \Delta e \) the single-particle energy spacing between the two top levels. A significant occupation of the first excited level occurs when \( k_BT \sim \delta \). Since we are assuming \( k_BT \ll \Delta e \), this implies \( \delta \ll \Delta e \). While in the CI model the probability for that to occur is small due to level repulsion, this is not so in the presence of exchange (i.e., \( \Delta e \sim 2J_s \) is much more likely than \( \Delta e \sim 0 \)).\(^{30}\) Second, at finite temperature the peak involvement changes the free energy of the QD upon adding a particle. Then, as we show below, the entropy contribution\(^{55–57}\) leads to a shift of the peak position that depends on the spin transition in the QD.

A. General approach

We now proceed with a detailed calculation. Let us consider the regime \( \Gamma \ll k_BT, \Delta \ll k_BT \), where \( \Gamma \) is the total width of a level in the QD. Near the CB peak corresponding to the \( N-1 \rightarrow N \) transition, the linear conductance is given by\(^{56,58,59}\)

\[
G(N) = \frac{e^2}{h} k_BT P^N \sum_a \frac{\Gamma_{a}^{L} \Gamma_{a}^{R}}{\Gamma_{a}^{L} + \Gamma_{a}^{R}} w_a \tag{38}
\]

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

\[
w_a = \sum_{j,i} F_{eq}(j|N) \langle \Psi_j^N | c_{\alpha,i}^\dagger | \Psi_{j-1}^N \rangle^2 \left[ 1 - f(\epsilon_j - \epsilon_i) \right]. \tag{39}\]

Here, (i) \( P^N \) is the equilibrium probability that the QD contains \( N \) electrons, (ii) \( \tilde{H}(QD)|\Psi_j^N \rangle = \epsilon_j |\Psi_j^N \rangle \) so that “\( j \)” labels the many-body states of the QD, (iii) \( F_{eq}(j|N) \) is the conditional probability that the eigenstate \( j \) is occupied given that the QD contains \( N \) electrons, and (iv) \( f(\epsilon) = \frac{1 + \exp[(-\epsilon - E_F)/k_BT]}{1 + \exp[(-\epsilon - E_F)/k_BT]} \). Since near the peak only the states with \( N-1 \) and \( N \) electrons are relevant, we have\(^{56}\)

\[
P^N_{eq} = \frac{\exp(-\Omega_N)}{\exp(-\Omega_N) + \exp(-\Omega_{N-1})} = f(\mathcal{F}_N - \mathcal{F}_{N-1}) \tag{40}\]

with \( \Omega_N = \mathcal{F}_N - \mu N \) and \( \mathcal{F}_N \) the canonical free energy of the QD. To make the dependence on \( N \) explicit, let us denote by \( \{E_j\} \) the eigenenergies of \( \tilde{H}(QD) \) without the charging energy term and define \( \delta N = (N - \frac{1}{2}) - N \). Then, \( \epsilon_j - \epsilon_i = E_j - E_i - 2E_{C} \delta N + 2E_{C} \delta N \).

\[
\mathcal{F}_N - \mathcal{F}_{N-1} = -k_BT \ln \frac{Z_N}{Z_{N-1}} = E_N - E_{N-1}
\]

\[
+ k_BT \ln \frac{F_{eq}(j|N)}{F_{eq}(j|N-1)} + 2E_{C} \delta N \tag{41}\]

with \( Z_N \) the canonical partition function. Note that Eq. (41) is valid for any \( i \) and \( j \). The contribution of the transition \( i \rightarrow j \) to the conductance reaches its maximum when \( f(\mathcal{F}_N - \mathcal{F}_{N-1})[1-f(\epsilon_j - \epsilon_i)] \) peaks, namely, when

\[
E_F = E_N - E_{N-1} + \frac{k_BT}{2} \ln \frac{F_{eq}(j|N)}{F_{eq}(j|N-1)} + 2E_{C} \delta N. \tag{42}\]

B. Ground-state-dominated transitions

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

\[
E_F = E_{GS} - E_{GS} - \frac{k_BT}{2} \ln \frac{2\delta_{GS} + 1}{2\delta_{GS}^{-1} + 1} + 2E_{C} \delta N. \tag{43}\]

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.\(^{55–57}\) Except for a factor \( \frac{1}{2} \) in front of the entropic term, Eq. (43) corresponds to replacing \( E_{GS} \) by \( \mathcal{F}_N \) in the usual condition for the peak position, which is what we would naively expect at finite temperature [this factor appears because Eq. (39) involves energy differences].

Because the rms of the PSD is \( \sim 0.3 \Delta \) (see Fig. 1), 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.\(^{56}\) While in the CI model this introduces only a constant shift between the even and odd distributions,\(^{64}\) 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 \( E_{GS}^0 \) 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.\(^{55,56}\) The reason is that \( F_{eq}(j|N) \), the overlap \( |\langle \Psi_j^N | c_{\alpha,i}^\dagger | \Psi_{j-1}^N \rangle|^2 \), and the value of \( P^N_{eq} \times [1-f(\epsilon_j - \epsilon_i)] \)
at its maximum depend on the particular spin transition involved. In the simplest case when only the GS is relevant, we get
\[ F_{eq}(f|N)\{p_{eq}^{N}[1-f(e_j-e_i)]\}_{max} = \frac{1}{(\sqrt{2S'+1} + \sqrt{2S+1})^2} \tag{44} \]

and
\[ \sum_{S'_z,S_z} |\langle \Psi_{S'_z}^\dagger |e_{\alpha,a} |\Psi_{S_z}^N \rangle|^2 = \begin{cases} 2S'+1 & \text{if } n_\alpha = 0, \\ 2S+1 & \text{if } n_\alpha = 1, \end{cases} \tag{45} \]

where \( S'(S) \) and \( S'_z(S_z) \) are the quantum numbers of the state with \( N(N-1) \) particles.\(^{62}\) At low temperature, most transitions correspond to the first case in Eq. (45) when \( S' > S \) and to the second when \( S' < S \). Using that, we finally get
\[ G_{\text{peak}} = \frac{2e^2}{\hbar k_BT} \frac{\Gamma_{\alpha}^L + \Gamma_{\alpha}^R}{\Gamma_{\alpha}^L + \Gamma_{\alpha}^R} \tag{46} \]

with
\[ \lambda = \frac{2(S'+S) + 3}{4(\sqrt{2S'+1} + \sqrt{2S+1})^2}. \tag{47} \]

Then, the average conductance peak depends not only on the average coupling to the leads but also on the probability of the transition \( S \rightarrow S' \)—i.e., it depends on \( J_S \) and on the statistics of the single-particle spectrum and so on magnetic field.

This is relevant for a quantitative understanding of the low-temperature behavior of \( \alpha = 1 -(G_{\text{peak}})_{\text{GOE}}/(G_{\text{peak}})_{\text{GUE}} \) in closed QD’s.\(^{53}\) 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—how 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 \( (k_BT \sim 0.4\Delta) \) in Ref. 63.\(^{64}\) Notice that both the CI model and dephasing processes lead to values smaller than 0.25.\(^{65–68}\)

**D. Several-states 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. (38) with respect to \( N' \). For arbitrary \( T \), this requires the calculation of all possible transitions between the eigenstates of \( \tilde{H}_{\text{QD}} \) with \( N' - 1 \) and \( N \) electrons. For simplicity, we restrict ourselves to low enough temperature so that only a few excited states are relevant.\(^{69}\) Therefore, we kept six states in the even case and four 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),

**FIG. 2.** Schematic representation of some low-energy states considered in the calculation of the PSD. The scheme at the top (bottom) corresponds to \( N \) even (odd). Below each state is shown its energy difference from the left most one within the CEI model. \( \Delta e_1 \) and \( \Delta e_2 \) are the first and second level spacings, respectively, 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 transitions lead to different spacings which in turn leads to a smearing of the PSD. Figure 2 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

**FIG. 3.** Top panel: Finite temperature CB peak spacing distribution corresponding to the CEI model [Eq. (1)] with \( J_S = 0.28\Delta \) (\( r_s = 1 \)) and \( k_BT = 0.3\Delta \). Notice that the \( \delta \) function in the odd distribution (solid line) is completely smeared out by temperature and that the even distribution (dashed line) develops a peak. Bottom panel: Same but neglecting the fluctuation of the coupling to the leads. Note that the long tail in the odd distribution (solid line) for large spacing is absent, and that the width of the peak in the even distribution is significantly reduced.

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52.4% and 39.6%, respectively, at \( k_B T = 0.3 \Delta \) and \( J_S = 0.28 \Delta \). In the odd case, the lowest states are those 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 nonzero temperature. Besides the expected smearing of the sharp features and their shift due to the entropic term in Eq. (43), there are two important new effects: (i) 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. (ii) 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 (it is shifted to the left since it essentially corresponds to \( S = 0 \) cases).

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 \( \Delta \epsilon_i = 2 J_S \) collapse into a single (average) value for the spacing, which leads to a peak in the PSD. According to Eq. (42) the corresponding CB peaks are shifted by \( \sim \pm \frac{1}{2} k_B T \ln(4/2) \), which gives a total shift of \( k_B T \ln 2 \) for the peak in the PSD. The fact that the \( \frac{1}{2} \rightarrow 0 \rightarrow \frac{1}{2} \) transition is shifted to the left while the \( \frac{1}{2} \rightarrow 1 \rightarrow \frac{1}{2} \) one is shifted to the right also contributes to the formation of the peak.

Note that the rms of the distribution is reduced by temperature. In fact, we find 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 \( \Gamma_\alpha = \text{cte.} \) 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. The two peaks, which are visible only in the absence of fluctuations, are caused by the same physics as the peak in the even distribution—the one to the right also contains some residual contribution from the \( \delta \) function. The absence of the long tail 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 \( S = \frac{1}{2} \): \( 0 \rightarrow \frac{1}{2} \rightarrow 0 \), \( 0 \rightarrow \frac{1}{2} \rightarrow 1 \), \( 1 \rightarrow \frac{1}{2} \rightarrow 0 \), and \( 1 \rightarrow \frac{1}{2} \rightarrow 1 \). The spacing in each case is \( J_S \), \( \Delta \epsilon_2 - J_S \), \( \Delta \epsilon_1 - J_S \), and \( \Delta \epsilon_1 + \Delta \epsilon_2 - 3 J_S \), respectively. It is easy to show that at \( T = 0 \), the conditions on \( \Delta \epsilon_1 \) and \( \Delta \epsilon_2 \) for each transition to occur, that is, for the GS to have the appropriate spin, leads to a spacing \( \approx J_S \) in all the cases. This result is a consequence of the “yes-no” conditions required at \( T = 0 \). At

\[
T \neq 0, \quad \text{those conditions are relaxed and the last three transitions can lead to a larger spacing (note also the shift due to the entropic effect). This thermal broadening is responsible for the disappearance of the \( \delta \) function. However, because the realizations contributing to that part of the distribution have \( \Delta \epsilon_i = 2 J_S \), 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 wave functions 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 \( k_B T \approx 0.3 \Delta \).

**E. Corrections to CEI model**

Results including the leading-order corrections are shown in Fig. 4 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 experi-
mental 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. 15 shows that this is indeed the case. In fact, the agreement between these data and the PSD shown in the lower panel of Fig. 4 is good, both qualitatively and quantitatively.

VIII. CONCLUSIONS

In this work we have calculated the Coulomb blockade peak spacing distribution including the most representative leading-order corrections (up to $\Delta/\sqrt{g}$) 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, but 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 $J_5$ and on many geometry-dependent parameters that could vary a bit for the actual QD. It could also be argued that the RPA approach used in the calculation of the screening of the Coulomb potential is not appropriate for $r_1 \sim 1$. 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 $J_5$. Such a renormalization, however, could have an important impact both on the shape of the distribution and on the strength of the even/odd effect since they are quite sensitive to the value of $J_5$. An experimental determination of $J_5$ should, then, be a high priority.

We find that scrambling and the gate effect are in general the dominant corrections. In order to emphasize the fluctuations of the interactions, however, one could introduce a top gate. Under such a condition, fluctuations would be dominated by the diagonal part of the Coulomb interaction since the contribution for the off-diagonal terms is negligible—only for small dots ($g \sim 1$) do the latter become important.

For $T \neq 0$ the picture is quite different. At $k_B T \sim 0.3 \Delta$, the roles of the even and odd distributions 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 rms 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 (i) 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 (ii) 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 clearly observable feature.

It is important to point out that our results do not explain the data of either Refs. 17 or 18. Nevertheless, in both cases there are some elements that suggest 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 $J_5 \sim 0.25 \Delta$. 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. (9) and (12) and lead to larger fluctuations of both $M_{a,b}$ and $X_{a,b}$. This subject is quite complex and we leave it for future work. Nevertheless it is important to mention that the rms in Ref. 18 is of order 0.4$\Delta$ and that there is a weak even/odd effect.

Finally, we would like to emphasize that low-$T$ experiments should be able to distinguish between the large dot ($g \gg 1$) and the small dot ($g \sim 1$) regimes. In the former, the PSD becomes dramatically sharper as temperature is decreased. In the latter, because the larger $T=0$ mesoscopic fluctuations lead to a Gaussian-like distribution, the PSD will remain featureless.

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APPENDIX A: THE DIFFUSIVE CASE

Similar results for the leading-order corrections can be obtained in the case of diffusive QD’s after the appropriate change of some definitions. First, the dimensionless conductance is now given by $g = h \gamma_1 / \Delta$ where $\gamma_1$ is the smallest nonzero eigenvalue of the diffusion equation, $-D \nabla^2 f_n (r) = \gamma_0 f_n (r)$, supplemented with von Neumann boundary conditions. $D = \nu \beta / 2$ is the diffusion constant and $t$ the mean free path. Second, $k(r_1,r_2) = \exp (-t / D f_0 (k_0 \beta r))$ with $r = |r_1 - r_2|$. Third, the propagator $\Pi_B (r_1,r_2)$ is replaced by its diffusive counterpart

$$\Pi_D (r_1,r_2) = \frac{\Delta A}{\pi} \sum_n f_n (r_1) f_n (r_2) \frac{1}{\hbar \gamma_n}. \quad (A1)$$

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

$$\gamma_{m,n} = \frac{D \beta^2}{R^2} \delta_{m,n}, \quad \beta'_{m,n} (\beta_{m,n}) = 0, \quad (A2)$$
and

\[ f_{m,n}(r) = A_{m,n} \begin{pmatrix} \cos m\phi \\ \sin m\phi \end{pmatrix} J_m \left( \frac{\beta_{m,n}}{R} \right) \]  

(A3)

with

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

(A4)

Here, \( J_m(x) \) is a Bessel function and \( f_{m,n}(x) \) its derivative. Note that the first nonzero eigenvalue, \( \gamma_{1,1} \), is proportional to the square of the first zero of \( J_1 \), \( \beta_{1,1} = 1.84 \). 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), \( f_{1,1}(r) \propto \cos \phi(\beta_{1,1}r/R) \). Then, \( g = hD \beta_{1,1}^2/4\Delta \propto l/R \sqrt{N} \). For \( N \sim 500 \) and \( l \sim R/2 \) this gives \( g \approx 13 \).

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

(A5)

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

2. Diagonal elements

In this case, the terms in Eq. (12) that involve \( k(r_1 - r_2) \) are small (assuming \( l \ll \sqrt{A} \)) and can be neglected. Then, \( \text{var}(M_{a,b}) = \Delta^2/2A^2 \int dr_1 dr_2 [\Pi_D(r_1, r_2)]^2 \).  

(A6)

Assuming a disc geometry we get \( \text{var}(M_{a,b}) = c_2 \Delta^2/4g^2 \) with

\[ c_2 = \frac{2}{\pi^2} \sum_{\gamma_{m,n}} \left( \frac{\gamma_{1,1}}{\gamma_{m,n}} \right)^2 = \frac{2}{\pi^2} \sum_{m=0}^{\infty} \sum_{n=1}^{\infty} \left( \frac{\beta_{1,1}}{\beta_{m,n}} \right)^4 = 0.26. \]  

(A7)

Once again, the numerical result is similar to the one we obtained for the ballistic case. For instance, using \( N \sim 500 \) and \( l \sim R/2 \), we get \( \text{rms}(M_{a,b}) = 0.020A \), which should be compared with the second row in Table 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 \( S = \frac{1}{2} \).

\[ E_{S=1/2}^{(2)} = \sum_{\beta > \alpha, \gamma \neq \beta} \frac{3|u_{\alpha, \beta, \gamma, \delta}|^2 + |a_{\alpha, \beta, \gamma, \delta}|^2}{e_{\alpha} + e_{\beta} - e_{\gamma} - e_{\delta}} \left( 1 - \frac{\delta_{\alpha, \beta}}{2} \right) \left( 1 - \frac{\delta_{\gamma, \delta}}{2} \right) + \sum_{\alpha \neq \beta, \gamma} \frac{3|u_{\alpha, \beta, \gamma, \delta}|^2 + |a_{\alpha, \beta, \gamma, \delta}|^2}{e_{\alpha} + e_{\beta} - e_{\gamma} - e_{\delta}} \left( 1 - \frac{\delta_{\alpha, \beta}}{2} \right) \left( 1 - \frac{\delta_{\gamma, \delta}}{2} \right) \]  

\[ + \sum_{\beta > \alpha, \gamma} \frac{3|u_{\alpha, \beta, \gamma, \delta}|^2 + |a_{\alpha, \beta, \gamma, \delta}|^2}{e_{\alpha} + e_{\beta} - e_{\gamma} - e_{\delta}} \left( 1 - \frac{\delta_{\alpha, \beta}}{2} \right) + \sum_{\beta > \alpha, \gamma} \frac{\Sigma_{\alpha \neq \beta} \rho(3u_{\alpha, \beta, \gamma, \delta} + a_{\alpha, \beta, \gamma, \delta})}{2(e_{\beta} - e_{\gamma})} \left( 1 - \frac{\delta_{\alpha, \beta}}{2} \right) + \frac{3}{4} |u_{\alpha, \beta, \gamma, \delta} + a_{\alpha, \beta, \gamma, \delta}|^2 \]  

\[ + \sum_{\beta > \alpha} \frac{|\Sigma_{\gamma} \rho(3u_{\alpha, \beta, \gamma, \delta} + a_{\alpha, \beta, \gamma, \delta})|}{16(e_{\beta} - e_{\gamma})}, \]  

(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 \( \Sigma' \) in which case the singly occupied level labeled “1” is included. Note that there are several terms which add coherently.


7. R. A. Jalabert, A. D. Stone, and Y. Alhassid, Phys. Rev. Lett. 68,


32 To be more specific, we refer to a QD as “typical” if (i) it has irregular shape, which guarantees a chaotic behavior for the classical dynamics and therefore RMT statistics for the single-particle properties; and (ii) its size (~500 nm) and electron density (~2×10^{13} cm^{-2}) guarantee both a large number of electrons (N~300) and weak interaction (r_e~1).


40 By using the Strutinsky method developed in Ref. 34 and local-density-matrix functional theory, it is possible to obtain both the direct and the exchange terms of the Coulomb interaction. Therefore, Eq. (4) is fully justified. T. T. Ong and H. U. Baranger (unpublished).


47 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.


49 One should note, however, that the covariance between the matrix elements M_{\alpha\beta} and M_{\gamma\delta} is of order \Delta^2/g^3 (see Ref. 48 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.

50 The latter would reduce both the gate effect and the scrambling. See Sec. V.


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


59 We assume that the occupation numbers \{n_\alpha\} are good quantum numbers. Namely, \langle [H_{QD}, n_\alpha]\rangle = 0.

60 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 ms(n_{\alpha\beta}) which is negligible.


62 The quantum numbers S and S_\parallel are not enough to specify a many-body state if the number of singly occupied levels is bigger than two, even for a given set \{n_\alpha\} of occupation numbers (see Ref. 51). In that case, additional quantum numbers k and k’ must be included in Eq. (45). This introduces an extra factor N_{\parallel}(N_{\perp}) for n_\alpha=0, n_{\parallel}=1 with N_{\parallel}(N_{\perp}) the degeneracy associated with k (k’).

Notice, however, that $\bar{\alpha}$ 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 comes first in the GOE case.


Because of 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 Figs. 3 and 4.

