

Interactions and interference in quantum dots: Kinks in Coulomb-blockade peak positions

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We investigate the spin of the ground state of a geometrically confined many-electron system. For atoms, shell structure simplifies this problem—the spin is prescribed by the well-known Hund’s rule. In contrast, quantum dots provide a controllable setting for studying the interplay of quantum interference and electron-electron interactions in general cases. In a generic confining potential, the shell-structure argument suggests a singlet ground state for an even number of electrons. The interaction among the electrons produces, however, accidental occurrences of spin-triplet ground states, even for weak interaction, a limit which we analyze explicitly. Variation of an external parameter causes sudden switching between these states and hence a kink in the conductance. Experimental study of these kinks would yield the exchange energy for the “chaotic electron gas.” [S0163-1829(99)51448-3]

The evolution of the properties of a system as a continuous change is made to it is a ubiquitous topic in quantum physics. The classic example is the evolution of energy levels as the strength of a perturbation is varied.¹ Typically, neighboring energy levels do not cross each other, but rather come close and then repel in an “avoided crossing.” However, if there is an exact symmetry, neighboring levels can have different symmetries uncoupled by the perturbation, and in this special case they can cross.

A new and powerful way of studying parametric evolution in many-body quantum systems is through the Coulomb-blockade peaks that occur in mesoscopic quantum dots.^{2–5} The electrostatic energy of an additional electron on a quantum dot—an island of confined charge with quantized states—blocks the flow of current through the dot—the Coulomb blockade.^{6,7} Current can flow only if two different charge states of the dot are tuned to have the same energy; this produces a peak in the conductance through the dot. The position of the Coulomb-blockade peak depends on the difference in ground state energy upon adding an electron, $E_{\text{gr}}(N+1) - E_{\text{gr}}(N)$. Thus, the evolution of the peak position reflects the evolution of these many-body energy levels as a parameter, such as magnetic field or shape distortion, is varied.

Since quantum dots are generally irregular in shape, the orbital levels have no symmetry and so avoid crossing. However, the spin degrees of freedom are often decoupled from the rest of the system, so states of different total spin can cross. Such a crossing will cause an abrupt change in the evolution of the Coulomb-blockade peak position—a kink—as the spin of the ground state changes, even though there is no crossing in the single-particle states. Such kinks have been observed in small circular dots—“artificial atoms”—because of their special circular symmetry.⁵ More

generally, kinks should occur in generic quantum dots with no special symmetries.⁸ In fact, the data of Ref. 4 show evidence for kinks in large dots, though they were not the subject of that investigation.

Small circular dots behave much like atoms (hence “artificial atoms”): the circular symmetry causes degeneracy of the orbital levels and so a large spacing between allowed energies. In sharp contrast, there is no degeneracy in irregular dots: the typical single-particle orbital level separation is simply given by $\Delta \equiv 1/\nu V$, where ν is the bulk density of states and V is the volume of the dot. Kinks in the evolution of Coulomb-blockade peak positions may occur whenever the ground state of the dot is separated from an excited state with different spin by an energy of order Δ . The interference effects causing the separation are unique to each state and change upon tuning. In fact, the two states may switch at a certain point, the former excited state becoming the ground state: such switching corresponds to a kink. Note that kinks occur in pairs: kinks in the peaks corresponding to the $N \rightarrow N+1$ transition, and that for $N-1 \rightarrow N$, both occur when $E_{\text{gr}}(N)$ switches. We see from this argument that kinks in the evolution of peak positions with parameter is a general property of quantum dots.⁸

Here we analyze these kinks explicitly in a particular limit. Consider a large quantum dot in which the single-particle properties are “random:” the statistics of the energies follow the classic random matrix ensembles⁹ and the wave functions obey Gaussian statistics with a correlation function given by the superposition of random plane waves.¹⁰ The single-particle properties of such random systems have been extensively investigated, and it has been conjectured, with considerable evidence, that these are good models for quantum dots in which the classical dynamics is chaotic.^{7,11}

To treat the Coulomb blockade, we must consider not only single-particle properties but interactions among the particles as well. One natural way to proceed is to treat these interactions in the basis of self-consistent single-particle states $\{\psi_m(\mathbf{r})\chi_\sigma(s)\}$, where m and σ are the labels of orbital and spin states, respectively, (we neglect the weak spin-orbit interaction). In the limit of zero interaction, two electrons occupy each filled orbital state, except for the top level when the total number of electrons is odd. Because of the interference produced by confinement in the dot, the electron density is not smooth but rather has small deviations from the classical-liquid result. Due to the electron-electron interaction, these deviations contribute to the ground-state energy, in addition to the conventional ‘‘classical-liquid’’ charging energy. If the interaction does not change the double occupancy of the levels, one finds that the part of such contribution coming from the last doubly occupied level n is

$$\xi_{n,n} \equiv \int d\mathbf{r}d\mathbf{r}' [|\psi_n(\mathbf{r})|^2 - \langle |\psi_n(\mathbf{r})|^2 \rangle] V_{\text{scr}}(\mathbf{r}-\mathbf{r}') \times [|\psi_n(\mathbf{r}')|^2 - \langle |\psi_n(\mathbf{r}')|^2 \rangle]. \quad (1)$$

It is appropriate to use the short-ranged screened interaction V_{scr} here since the smooth background of the other electrons provides screening; $\langle \dots \rangle$ denotes the standard ensemble averaging. If, because of the interactions, one of the electrons of that level is promoted to the next orbital state, the result (1) is modified to become

$$\xi_{n,n+1}^\pm \equiv \int d\mathbf{r}d\mathbf{r}' [|\psi_n(\mathbf{r})|^2 - \langle |\psi_n(\mathbf{r})|^2 \rangle] V_{\text{scr}}(\mathbf{r}-\mathbf{r}') \times [|\psi_{n+1}(\mathbf{r}')|^2 - \langle |\psi_{n+1}(\mathbf{r}')|^2 \rangle] \pm \int d\mathbf{r}d\mathbf{r}' \psi_n(\mathbf{r}) \psi_{n+1}^*(\mathbf{r}) \times V_{\text{scr}}(\mathbf{r}-\mathbf{r}') \psi_n^*(\mathbf{r}') \psi_{n+1}(\mathbf{r}'). \quad (2)$$

The signs $+$ and $-$ in Eq. (2) correspond to the singlet and triplet states, respectively. The Hartree-Fock approach of Eqs. (1) and (2) is valid if the interactions are not too strong and is expected to be relevant for the experimental semiconducting and metallic quantum dots.

For a large ballistic dot, $k_F L \gg 1$, the lack of correlation among the random wave functions ψ_n and ψ_m with $n \neq m$ leads to a hierarchy of the matrix elements of the interaction¹² (here k_F is the Fermi wave vector of electrons in the dot, and L is the linear size of the dot). The first integral in Eq. (2) vanishes in the limit $k_F L \rightarrow \infty$, and one is left only with the second, exchange interaction, term. In the same limit, the exchange interaction term has a nonzero average value and vanishingly small mesoscopic fluctuations. The lowest of two energies $\xi_{n,n+1}^\pm$ corresponds to the triplet state ($\pm \rightarrow -$). Neglecting the small mesoscopic fluctuations of the energies $\xi_{n,n}$ and $\xi_{n,n+1}^-$, one finds the difference between the energies of the singlet state formed by doubly occupied levels, and of the triplet state with two singly occupied orbital levels:

$$\xi \equiv \langle \xi_{n,n} \rangle - \langle \xi_{n,n+1}^- \rangle = 2 \int \frac{d\mathbf{r}d\mathbf{r}'}{V^2} V_{\text{scr}}(\mathbf{r}-\mathbf{r}') |F(\mathbf{r}-\mathbf{r}')|^2 = \frac{2}{V} \overline{\hat{V}_{\text{scr}}(\mathbf{k}-\mathbf{k}')}. \quad (3)$$

Here $F(\mathbf{r}) \equiv \overline{\exp(ik'\mathbf{r})}$, with the bar denoting the average over the Fermi surface $|\mathbf{k}'| = k_F$, and V is the volume of the dot.

In the above argument, we have implicitly assumed the absence of time-reversal symmetry. For $B=0$, the same basic argument holds, but the interaction in the Cooper channel should be included; this increases ξ making the proportionality constant in Eq. (3) larger than 2.

We thus consider a model¹³ with a single nonzero interaction constant ξ . This quantity is simply related to the usual electron gas parameter r_s (the ratio of the Coulomb energy at the mean interparticle distance to the Fermi energy): $\xi \approx (1/\sqrt{2}\pi)r_s \ln(1/r_s)\Delta$ for small r_s in two dimensions and in the absence of time-reversal symmetry. As r_s increases, the considerations discussed here apply until $\xi \gtrsim \Delta$ at which point the Stoner criterion for a magnetic instability is approached. For instance, for $r_s=1$, averaging the Thomas-Fermi screened potential over the Fermi surface yields $\xi = 0.6\Delta$ in two dimensions.

The distribution of electrons among the levels depends on the single-particle level spacing compared to ξ . This is particularly clear when the total number of electrons N is even: the top two electrons can either be in the same orbital level at a cost of ξ in interaction energy or one can be in level $N/2$ and the other in $N/2+1$ at an energy cost of $\epsilon_{N/2+1} - \epsilon_{N/2}$. Since the magnitudes of both ξ and $\epsilon_{N/2+1} - \epsilon_{N/2}$ are of order Δ , sometimes the top level is doubly occupied and sometimes not. In the case of double occupation, the state is, of course, a singlet; if two sequential levels are occupied, the exchange interaction leads to a triplet state. If at most two orbital levels are singly occupied, the ground state energy of a dot is, then, a sum of three terms:

$$E_{\text{gr}} = E_{\text{ch}} + \sum_{(n,\sigma) \text{ filled}} \epsilon_{n,\sigma} + M\xi, \quad (4)$$

where M is the number of doubly occupied levels. For our arguments, the number of electrons is constant and so the charging energy E_{ch} is irrelevant. Note that the energy (4) is equivalent to the simultaneous filling of two sequences of levels, one of which is rigidly shifted by ξ from the other.¹³ Finally, if several orbital level spacings in sequence are small, more complicated configurations occur for both even and odd N .^{14,15} Moreover, the problem of the ground-state spin of a mesoscopic system becomes very complicated upon approaching the Stoner instability.¹⁵

As a parameter is varied, the single-particle energies change and may cause a change in the level occupations and so a kink. This is explained and illustrated in Fig. 1. The parameter involved could be, for instance, an applied magnetic field or a gate voltage which changes the shape of the dot.

The distribution of the kinks in the parameter space follows from a random matrix model. We assume that the Hamiltonian of the dot follows the Gaussian orthogonal en-

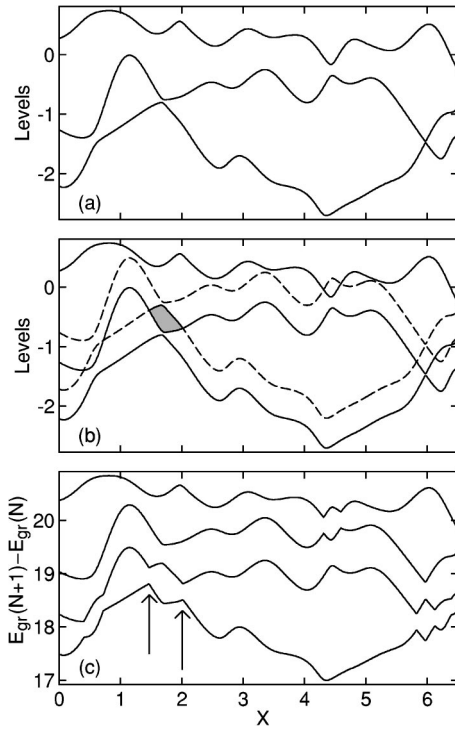


FIG. 1. Mechanism for kinks in the Coulomb-blockade peak positions: Gaussian process simulation results as a function of scaled parameter x ($\beta=2$). (a) Three typical orbital energy levels; note the infrequent avoided crossings. (b) Two sets of energy levels, one for singly occupied orbitals (solid) and the second for double occupancy (dashed). For a large dot, the doubly occupied levels are rigidly shifted from those for single occupancy by the interaction ξ ($=0.5\Delta$ here), see Eq. (4). Consider an even number of electrons in which the top two particles are placed in the levels shown. When the doubly occupied state (first dashed line) has higher energy than the next orbital level (second solid line), the ground state has two partially occupied levels—a triplet spin state. When these two levels cross, the lowest energy in the triplet sector crosses the lowest singlet state. (c) Difference in energy upon adding an electron, proportional to the Coulomb-blockade peak position. Traces offset by $\sim -E_{\text{ch}}$ for clarity. Crossings of the singlet and triplet levels cause kinks in the peak positions (arrows mark two examples). Two adjacent peaks are affected by each change in a ground state: they have kinks at the same x and switch which orbital level they are tracking.

semble in the absence of a magnetic field (GOE, $\beta=1$) and the Gaussian unitary ensemble for nonzero B (GUE, $\beta=2$).⁹ The dependence on the parameter X is included by means of a Gaussian process;^{16,17} we consider the process

$$H(X) = H_1 \cos(X) + H_2 \sin(X), \quad (5)$$

where the distributions of H_1 and H_2 follow the appropriate Gaussian ensemble. Extensive work on parametric correlations has shown that the properties of Gaussian processes are universal when the energy is measured in units of the mean level separation Δ and the parameter is scaled by the typical rate at which energies are perturbed, $\langle (d\epsilon/dX)^2 \rangle^{1/2}$.^{16–18} The two scaled variables are ξ/Δ and $x \equiv X \langle (d\epsilon/dX)^2 \rangle^{1/2} / \Delta$. For simplicity, we restrict our attention to kinks caused by a change in configuration of the top two electrons when N is even.

The first quantity to consider is the mean density of kinks, ρ_{kink} . First, because a kink occurs when $\epsilon_{N/2+1} - \epsilon_{N/2} = \xi$, this density is proportional to the probability of having such a level separation. Second, ρ_{kink} must reflect the rate at which the levels change as a function of parameter. In fact, it is known that the distribution of the slopes of the levels, $d\epsilon/dX$, is Gaussian and independent of the distribution of the levels themselves.¹⁶ Thus, the two contributions are simply multiplied:

$$\rho_{\text{kink}} = \frac{2}{\sqrt{\pi}} p_{\epsilon}^{(\beta)}(\xi/\Delta) \left\langle \left(\frac{d\epsilon}{dX} \right)^2 \right\rangle^{1/2} \propto \xi^{\beta} \quad \text{for small } \xi, \quad (6)$$

where $p_{\epsilon}^{(\beta)}(s)$ is the distribution of nearest-neighbor level separations, for which the Wigner surmise⁹ is an excellent approximation. ρ_{kink} has a strong dependence on β when ξ is small because of the symmetry dependence of $p_{\epsilon}^{(\beta)}$, and so will be sensitive to a magnetic field. In fact, *the sensitivity to magnetic field could be used to extract experimental values for ξ in quantum dots—a direct measure of the strength of interactions.*

Next, an important property is the spacing in X between two neighboring kinks. For $\xi \ll \Delta$, kinks occur when two orbitals come very close and so are caused by avoided crossings of single-particle levels. Since each avoided crossing produces two kinks, kinks will occur in pairs, with small intrapair and large interpair separations. The behavior near an avoided crossing is dominated by just two levels and characterized by three parameters—the mean and difference of the slopes far from the crossing and the smallest separation. Wilkinson and Austin have derived the joint probability distribution of these parameters for Gaussian random processes.¹⁶ By expressing the intrapair separation in terms of these parameters and integrating over the joint distribution, we find that the distribution of intrapair separations is

$$P_{\text{intra}}(x) = 2x \left(\frac{\Delta}{\xi} \right)^2 \int_0^{(\xi/x\Delta)^2} du \exp(-u) \times \begin{cases} u^2, & \beta=2 \\ u^{3/2} [1 - u(x\Delta/\xi)^2]^{-1/2} / \sqrt{\pi}, & \beta=1. \end{cases} \quad (7)$$

For small x , P_{intra} is linear in the separation x both with and without a magnetic field.

The separation between pairs is usually large for small ξ —avoided crossings with small gaps are rare—typically many correlation lengths. Hence, there is no correlation between pairs: $P_{\text{inter}}(x)$ is Poisson (exponential) for large x . Correlation suppresses the probability of two close crossings. We make a simple model for this by assuming $P_{\text{inter}} \propto x$ for $x < x_0$ and so approximate P_{inter} by

$$P_{\text{inter}}(x) = \frac{C}{\alpha} \begin{cases} \exp[-(x-x_0)/\alpha], & x > x_0 \\ x/x_0, & x < x_0, \end{cases} \quad (8)$$

where C is for normalization. x_0 should be of order 1 in scaled units; we choose it to be the minimum of the correlation function of $d\epsilon/dx$, $x_0 = 0.85$ (0.6) for GOE (GUE). The mean density Eq. (6) sets α ,

$$1/\rho_{\text{kink}} = \langle x \rangle = \frac{1}{2} [\langle x \rangle_{\text{intra}} + \langle x \rangle_{\text{inter}}], \quad (9)$$

combined with the distribution P_{intra} . In this way we have a parameter-free expression for the distribution of the separation between adjacent kinks.

While the above theory is for $\xi \ll \Delta$, in the experiments,^{4,5} $r_s \sim 1$ so that $\xi \approx \Delta$. Hence, we turn to numerical calculation to test the range of validity of our expressions. Gaussian processes were produced using the Hamiltonian (5) with matrix size 200 over the full interval $x \in [0, 2\pi]$; the middle third of the spectrum was used. Sample energy levels for $\beta = 2$ are shown in Fig. 1.

Figure 2 shows the distribution of kink spacings for the experimentally relevant value $\xi = 0.5\Delta$ and $\beta = 1, 2$. Though outside the regime of immediate applicability, the theoretical curves agree closely with the numerical data. Thus the simple two-level calculation captures the main features of the kink distribution for $\xi \lesssim \Delta$ and so is adequate for describing experiments in large dots.⁴ Note that the pairing of kinks can help to distinguish them from simple avoided crossings in experimental traces.

Finally, the results here are based on two main approximations, the Hartree-Fock starting point and the neglect of fluctuations in the interaction energies $\xi_{n,m}$. While the former is strictly justified only for weak interactions, it is widely used and gives reasonable results if the interactions are not too strong ($r_s \sim 1$). Fluctuations will become important in small dots for which the spatial integrals in Eqs. (1) and (2) produce less averaging; in this case, a distribution of ξ should be incorporated. Relaxing either of these assumptions will change our quantitative predictions but will not change the main qualitative features.

In conclusion, through the properties of kinks in the Coulomb-blockade traces, experiments on quantum dots can directly determine the main interaction parameter in these dots and so obtain the exchange energy for the chaotic electron gas.

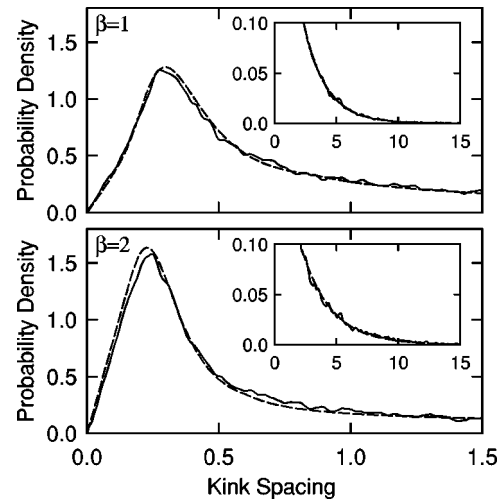


FIG. 2. Distribution of the separation between nearest-neighbor kinks in the Coulomb-blockade peak positions. The interaction strength is $\xi = 0.5\Delta$. Top: zero magnetic field (time-reversal symmetry, $\beta = 1$). Bottom: nonzero magnetic field ($\beta = 2$). Insets: tails of the distributions. Both the analytic theory for small ξ (dashed line) and the results of Gaussian process simulations (solid line) are shown. The excellent agreement is remarkable considering that $\xi = 0.5\Delta$ is not small and the absence of any fitting parameter.

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