Effects of spin and exchange interaction on the Coulomb-blockade peak statistics in quantum dots

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We derive a closed expression for the linear conductance through a quantum dot in the Coulomb-blockade regime in the presence of a constant exchange interaction. With this expression we calculate the temperature dependence of the conductance peak-height and peak-spacing statistics. Using a realistic value of the exchange interaction, we find significantly better agreement with experimental data as compared with the statistics obtained in the absence of an exchange interaction.

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The conductance through a quantum dot that is weakly coupled to leads displays sharp peaks as an applied gate voltage is varied. Each conductance peak describes the addition of one more electron into the dot, and between peaks the conductance is “blocked” by the Coulomb interaction. The statistics of both peak heights and peak spacings in dots for which the single-electron dynamics is chaotic have been intensively studied in recent years [1]. Some of the experimental observations, e.g. the peak-height distributions at low temperature [2, 3, 4], could be explained at least qualitatively by the constant-interaction (CI) model, in which the interaction is represented in the simple form of an electrostatic charging energy. Other measured observables, such as the peak-spacing distribution [1], have indicated that spin and residual interactions beyond the charging energy should be taken into account. A consistent theoretical approach that provides quantitative agreement with both the measured peak-height and peak-spacing statistics is still lacking.

Recently, a universal Hamiltonian was derived [6, 7] for a dot with a large Thouless conductance $g_T \sim VN$ ($N$ is the number of electrons). An important contribution to the interaction part of this Hamiltonian is a constant exchange interaction in addition to the usual charging-energy term. The remaining interaction terms are suppressed at large $g_T$. Here we study the effect of the exchange interaction on the finite-temperature statistics of both peak heights and spacings. To this end, we derive a closed expression for the conductance in the presence of a constant exchange interaction (in the sequential-tunneling limit). This formula expresses the conductance in terms of quantities that characterize spinless non-interacting electrons. We then calculate the finite-temperature peak-height and peak-spacing statistics and find them both to be sensitive to the exchange interaction. Using an RPA estimate of the exchange interaction for the samples studied experimentally in Refs. [5, 8], we obtain very good agreement with the observed temperature dependence of the standard deviation of the peak spacing. We also explain most of the known discrepancies between the experimental peak-height statistics and the predictions of the CI model for $kT \lesssim 0.6 \Delta$ ($\Delta$ is the mean spacing between spin-degenerate levels).

The universal Hamiltonian of a quantum dot in the limit $g_T \to \infty$ is given by

$$
\hat{H} = \sum_{\lambda \sigma} \epsilon_\lambda a_\lambda^\dagger a_\lambda + \frac{e^2}{2C} \hat{n}^2 - J_s \hat{S}^2,
$$

where $\epsilon_\lambda$ are spin-degenerate single-particle levels ($\sigma = \pm 1$ labels the spin). The second term in Eq. (1), where $C$ is the dot’s capacitance and $\hat{n}$ is the total–particle-number operator, accounts for the electrostatic energy of the dot. The third term, in which $\hat{S}$ is the total spin operator, describes a constant exchange interaction with strength $J_s$. The occupation-number operator $\tilde{n}_\lambda = \tilde{n}_{\lambda+} + \tilde{n}_{\lambda-}$ of any single-particle orbital $\lambda$ commutes with the total spin, $[\tilde{n}_\lambda, \hat{S}] = 0$, and the Hamiltonian $\hat{H}$ is invariant under spin rotations. Thus the eigenstates of $\hat{H}$ are characterized by their particle number $N$, the configuration of orbital occupation numbers $\mathbf{n} = \{n_\lambda\}$ ($n_\lambda = 0, 1$ or 2), the total spin $S$, and the spin projection $S_z = M$. We label the eigenstates as $|Nn_\gamma SM\rangle$ where the quantum number $\gamma$ distinguishes between states with the same total spin $S$ and particle configuration $\mathbf{n}$. The eigenenergies are given by

$$
\epsilon_{\mathbf{n}\gamma} = \sum_\lambda \epsilon_\lambda n_\lambda + e^2 N^2/2C - J_s S(S+1).
$$

In the limit of sequential tunneling (when a typical tunneling width is small compared with $kT$ and $\Delta$), the conductance can be calculated using a rate-equations approach. In Ref. [9] we developed such an approach in the presence of interactions and spin. In particular, an explicit solution exists when the orbital occupation numbers $n_\lambda$ are good quantum numbers. Expressing the conductance $G$ in a rescaled form $G = (e^2\tilde{\Gamma}/8\hbar kT)g$ (where $\tilde{\Gamma}$ is an average width of a level), we have, in the vicinity of the $N+1$-st Coulomb-blockade peak

$$
g = 4 \sum_{\mathbf{n}\gamma S} \tilde{\Gamma}_{\mathbf{n}\gamma S}^0 f(\epsilon_{\mathbf{n}\gamma S}/\bar{\Delta}) |\langle \mathbf{n}|\mathbf{n}\gamma S\rangle|^2 g_\lambda. \quad (2)
$$

Here $g_\lambda = 2\tilde{\Gamma}^{-1}\Gamma_\lambda/(\Gamma_\lambda + \Gamma_\lambda^{\dagger})$ are the single-particle level conductances, where $\Gamma_\lambda^{\dagger}$ are the partial widths of
an electron in orbital \( \lambda \) to decay to the left or right lead. The probability of finding the dot to be in the state \( |Nn\gamma SM\rangle \) is \( \tilde{P}^{(N)}_{nS} = e^{-\beta(\epsilon^{(N)}_{nS} - \epsilon_F N)|Z|} \), where the partition function \( Z \) is a Boltzmann-weighted sum over all possible \( N \)- and \((N+1)\)-body states (no other particle numbers contribute because of the charging energy), and \( \epsilon_F = \epsilon_c V_g + \epsilon_F \) is an effective Fermi energy (\( \epsilon_F \) is the Fermi energy in the leads, \( V_g \) is the gate voltage and \( \epsilon_c \) is the dot-gate capacitance). The Fermi-Dirac function \( f(x) = (1 + e^{\beta x})^{-1} \) is evaluated at an electron energy (relative to the Fermi energy) \( \epsilon^{(N)}_{nS} = \epsilon^{(N)}_{nS'} - \epsilon^{(N)}_{nS} - \epsilon_F \) that conserves energy at the transition between states \( |Nn\gamma SM\rangle \) and \(|(N+1)n'S'M'\rangle \). The corresponding reduced matrix element \( \langle (N+1)n'S'M'|a_{\lambda}^\dagger|Nn\gamma S\rangle \) enforces the selection rule \( S' = |S \pm 1/2| \).

Eq. (2) can be rewritten in the form
\[
g = \sum_\lambda (w^{(0)}_\lambda + w^{(1)}_\lambda) g_\lambda ,
\]
where the contributions with \( n_\lambda = 0 \) and \( n_\lambda = 1 \) are collected in \( w^{(0)}_\lambda \) and \( w^{(1)}_\lambda \), respectively. For the cases with \( n_\lambda = 0 \), the final \((N+1)\)-particle state is given by \(|(N+1)n'S'M') = \sum_{M_S}(SM\lambda^\dagger'S'M)\langle a_\lambda|Nn\gamma SM\rangle |Nn\gamma SM\rangle \), where \( (SM\lambda^\dagger'S'M) \) is a Clebsch-Gordon coefficient. When \( n_\lambda = 1 \) (and hence \( n_\lambda' = 2 \)), the \( N\)-particle state can be similarly related to the \((N+1)\)-particle state by changing to a hole representation. This leads to the following reduced matrix elements,
\[
(\gamma S'|a_{\lambda}^\dagger|\gamma S\rangle = (-)^{S-S'-1/2}\sqrt{2S'+1} \quad \text{if} \quad n_\lambda = 0, \\
\sqrt{2S+1} \quad \text{if} \quad n_\lambda' = 2.
\]
Using the relation \( \tilde{P}^{(N)}_{nS} f(\epsilon^{(N)}_{nS}) = \tilde{P}^{(N+1)}_{nS'}[1-f(\epsilon^{(N)}_{nS})] \), we get
\[
w^{(1)}_\lambda = 4 \sum_{S} \lambda_{N,S} P_{N,S} \sum_{S' = S \pm 1/2} \beta \sum_{S' = S \pm 1/2} (2S' + 1) f(\epsilon^{(N)}_{nS}) ,
\]
where \( \lambda_{N,S} \) is the particle-number operator of a non-degenerate orbital \( \lambda \). The function \( b_{\lambda_{N,S}} \) from Eq. (5b) is expressed by replacing \( \tilde{n}_\lambda \) by \((1 - \tilde{n}_\lambda) \) in Eq. (6). The complete expression for the conductance is then obtained from Eqs. (3), (4), (5), (6), (7) and the relation indicated in the previous sentence. Thus the dot’s conductance in model (1) is determined in terms of the free energy \( \tilde{F}_q \) and single-particle occupation numbers \( \tilde{n}_\lambda \).

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of \( q \) non-interacting spinless fermions. Both \( \tilde{F}_q \) and \( \langle \tilde{n}_\lambda \rangle \) are familiar from earlier works in the framework of the CI model, and can be expressed in closed form using particle-number projection [see Eqs. (140) in Ref. (1)].

In chaotic dots, the single-particle Hamiltonian in (1) is described by random-matrix theory. We have studied the statistics of peak heights and spacings for both the orthogonal and unitary symmetries. The dimension
of the configuration sum in Eq. (2) increases combinatorially with the number of single-particle orbitals and a direct use of (2) becomes impractical at higher temperatures. In contrast, the closed expression we derived greatly facilitates the calculation of the conductance for a rather large model system of 50 single-particle orbitals \( \lambda \). We checked that our results are not affected by the finite size of the system up to temperatures of \( kT \sim 3 \Delta \).

Theoretical calculations of the width \( \sigma(\Delta_2) \) of the peak-spacing distribution, based on a spinless CI model [8], describe qualitatively the observed decrease of this quantity with increasing temperature [5]. However, a proper modeling of the peak-spacing distribution itself requires the inclusion of spin. When spin is included and in the absence of an exchange interaction, the calculated values of \( \sigma(\Delta_2) \) show a large discrepancy with the experimental values (symbols). Fig. 2 also shows \( \sigma(\Delta_2) \) for non-zero values of \( J_s \). For a gas constant of \( r_s \sim 1.2 \) (that corresponds to the samples used in the experiments), the RPA estimate is \( J_s \approx 0.3 \Delta \) [8], and we find for this value a very good agreement with the measurements. The results for \( J_s = 0.5 \Delta \) underestimate the experimental widths. We remark that at temperatures \( kT \lesssim 0.4 \Delta \), the model [8] does not describe well the shape of the peak-spacing distribution, and it is necessary to include the fluctuating part of the universal Hamiltonian to explain the absence of bimodality [12, 13]. At higher temperatures, the bimodality is absent already in model [8] and the residual interaction has a negligible effect on the width.

Another measured quantity is the ratio between the standard deviation \( \sigma(g_{\text{max}}) \) and the average \( \bar{g}_{\text{max}} \) of the peak heights \( g_{\text{max}} \) [8]. The experimental data for this ratio (symbols in Fig. 2) are seen to be suppressed in comparison with the results of model [8] without an exchange term (long-dashed line in the left panel of Fig. 3). Spin-orbit interaction was proposed as a mechanism for this suppression at low temperatures [4]. It was necessary to assume a spin-orbit coupling that is sufficiently strong to completely decorrelate the spin-up and spin-down levels. However, spin-orbit effects are likely to be suppressed in the small dots used in the experiment. To determine whether an exchange interaction can explain the observed suppression of \( \sigma(g_{\text{max}})/\bar{g}_{\text{max}} \), we calculated this ratio versus temperature \( kT \) for different strengths of the exchange interaction (see Fig. 4). In the elastic limit (left panel), a realistic exchange interaction of \( J_s = 0.3 \Delta \) leads to closer agreement with the data. The remaining small discrepancy at temperatures \( kT \lesssim 0.6 \Delta \) can probably be accounted for by adding a realistic weak spin-orbit interaction. It still remains to explain the discrepancy at higher temperatures, where inelastic scattering may play a role. The calculation of Ref. [8] showed that the suppression of \( \sigma(g_{\text{max}})/\bar{g}_{\text{max}} \) due to inelastic scattering is small for \( J_s = 0 \). In the right panel of Fig. 2 we show results for the rapid-thermalization limit of strong inelastic scattering in the presence of an exchange interaction. While the agreement (for \( J_s = 0.3 \Delta \)) is now better at low temperatures, we do not expect inelastic scattering to be important at these temperatures. At higher temperatures, the rapid-thermalization limit does not describe the data, and it would be interesting to determine the effect of an additional weak spin-orbit term.

For \( kT \ll \Delta \) and \( J_s = 0 \), the peak-height distribution \( P(g_{\text{max}}) \) can be calculated analytically [6] and is shown for the unitary symmetry as a solid line in the left panel of Fig. 3 (compared to the case of spinless electrons, the peak heights are rescaled [8] by \( 8(\sqrt{2} - 1)^2 \approx 1.37 \)). Also shown (histogram) is the peak-height distribution calculated at \( kT = 0.01 \Delta \) and \( J_s = 0.5 \Delta \). No significant
interaction and found a significantly better quantitative agreement with experiment than in the absence of an exchange interaction.

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