Deformation of Quantum Dots in the Coulomb Blockade Regime

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We extend the theory of Coulomb blockade oscillations to quantum dots which are deformed by the confining potential. We show that shape deformations can generate sequences of conductance resonances which carry the same internal wavefunction. This fact may cause strong correlations of neighboring conductance peaks. We demonstrate the relevance of our results for the interpretation of recent experiments on semiconductor quantum dots.

73.23.Hk, 73.50.Bk, 73.40Gk

Recently two experimental groups have reported the first measurements of the distribution of Coulomb blockade peak heights in semiconductor quantum dots [1,2]. These measurements were designed to test various predictions of the statistical theory of the Coulomb blockade [3]. This theory was formulated by Jalabert, Stone and Alhassid for the low temperature regime $kT < \Delta$, where $\Delta$ is the mean resonance spacing. In this regime, transport through the quantum dot occurs by resonant tunneling through a single quasibound state. On the basis of a random matrix assumption for the quasibound eigenfunctions of the dot, the statistical distribution of the peak heights of the conductance resonances was derived [3] both for systems with time-reversal symmetry (vanishing magnetic field) and for systems with broken time-reversal symmetry (with sufficiently large magnetic field).

In the experiments [1,2], good agreement was found with the predicted form of the distribution functions. At the same time, unexpected correlations were observed [3] between neighboring peak heights. The correlations comprised up to four adjacent peaks. Even stronger correlations have recently been found in a set of experiments [4] addressing the phase of the transmission amplitude through a quantum dot. In these experiments, more than 10 consecutive conductance peaks displayed the same phase, and nearly the same peak height. This phenomenon has not been explained so far.

In this paper we propose a novel mechanism which can account for the above-mentioned correlations. It applies whenever the same set of capacitively coupled gate electrodes is used to define the depth and shape of the dot confining potential. This is the case in the experiments of Refs. [1,2,4] but not for others using a back gate. We study the effect of a deformation of the potential on the eigenvalues and eigenfunctions of the dot.

Several authors [3] have shown that a parabolic potential is a useful approximation to the confining potential of a quantum dot. To simplify the argument, we start with this case. We identify sequences of conductance resonances which, as a result of level crossings, carry the same internal wave function. Similar sequences are found if the parabolic potential is replaced by a more realistic confinement potential with level repulsion and chaotic classical electron motion. We first disregard the charging energy of the dot but show later that our conclusions remain essentially unchanged when this energy is included.

We choose the $x$ axis through the center and in the direction of transmission through the dot. To account for anisotropies imposed by the external gate potential (gp), we choose different values for the frequencies $\omega_x, \omega_y$ of the parabolic confining potential. For simplicity, we keep the frequency $\omega_x = \omega^0$ fixed and change the frequency $\omega_y = \omega^0(1 - \beta)$, with $0 \leq \beta < 1$. Increasing $\beta$ widens the potential in the $y$-direction and thus deforms it. Fig. 1 shows part of the single-particle spectrum versus $\beta$. The shell structure at $\beta = 0$ is clearly visible. The energy levels form a network of intersecting straight lines. Some lines run nearly parallel to the $\beta$-axis while others have large negative slopes. The explanation is simple. Each single-particle state is characterized by two quantum numbers $(n_x, n_y)$. States with small (large) values of $n_y$ have small (large) negative slopes. When two lines cross, the quantum numbers are carried along the

![FIG. 1. Energy levels of the two-dimensional harmonic oscillator with frequencies $\omega_x = 1$ and $\omega_y = 1 - \beta$ as functions of $\beta$.](image-url)
straight lines. We show below that the pattern in Fig. 1 is generic and applies also to the single-particle spectrum of deformed non-integrable potentials, with one difference. The points of intersection of the straight lines disappear and are replaced by avoided (Landau-Zener) crossings.

To present the essence of our argument, we replace Fig. 1 by an idealized picture (Fig. 2): A set of equally spaced straight lines (A-levels) runs parallel to the $\beta$-axis, a second similar set (B-levels) has large negative slope. To model the generic case, we have replaced actual crossings by avoided crossings. Single-particle wave functions retain their identity across avoided crossings in nearly the same way as if the lines were to intersect. Therefore, the wave function on any A-level is nearly independent of $\beta$, and so is the Fermi energy $E_F$ marked by a dashed line. At a fixed value of $\beta$, all single-particle states up to $E_F$ are filled. A change of the gp (and, therefore, of $\beta$) is slow on the scale of characteristic times of the quantum dot. Therefore, electrons in occupied orbitals follow the deformation $\beta$ adiabatically. Let $\delta\beta$ be the distance between B-lines, and gp$_{\bar{\beta}}$ be the change of the gp needed to change $\beta$ into $\beta + \delta\beta$. What happens as we increase the gp by gp$_{\bar{\beta}}$? The last occupied A-level moves adiabatically one “floor” down to its nearest analogue, thereby changing its wave function. The A-level right below $E_F$ becomes empty. If gp$_{\bar{\beta}} = \text{g}p_e$, the change of the gp needed to pull another electron into the dot, then the next conductance resonance will carry the very same single-particle state as its predecessor. (The Figure simplistically suggests that the next resonance occurs whenever a solid line crosses $E_F$; in reality the criteria given in (iii) apply). This process can repeat itself for a second, third, etc. time. Thus, subsequent conductance peaks might not be independent, but would be manifestations of one and the same single-particle state.

(i) To construct a more realistic case without the regularity of Figs. 1 and 2, we consider the two-dimensional single-particle Hamiltonian

$$H = \frac{\partial^2}{2m} + \frac{m\omega^2}{2}(x^2 + (1 - \beta)^2y^2) - \lambda \hbar \omega L^2,$$

where $L = i(y \frac{\partial}{\partial x} - x \frac{\partial}{\partial y}$ is the dimensionless $z$-component of the angular momentum operator. In nuclear physics, the three-dimensional analogue of $H$ is known as the Nilsson model and has been quite successful in explaining the spectra of deformed nuclei [9]. For $\beta > 0$ and $\lambda \neq 0$, $H$ is not integrable [6] and displays level repulsion. We may view $H$ as a mean-field approximation to the total Hamiltonian. The latter contains both, the mutual interaction of the electrons and the real confining potential. Any such approximation should lead to more or less chaotic single-particle motion.

Fig. 3 shows part of the spectrum of $H$ versus $\beta$. For $\beta = 0$ the eigenvalues $m$ of $L$ are good quantum numbers. The levels with $m \neq 0$ are pairwise degenerate. They form ascending sequences with $\pm m, \pm (m - 2), \ldots, \pm 1$ or 0. For $\beta > 0$, each eigenfunction contains a superposition of $m$-values. Depending on the strength $\lambda$, the mixing may extend over $m$-values from different shells. The overall pattern is quite similar to Fig. 1. The resolution in Fig. 3 is not fine enough to show that all crossings are avoided crossings. But is it realistic to assume that wave functions on (nearly) horizontal levels retain their identity when $\beta$ is changed? This, after all, is the central point used in our argument. We have inspected the eigenvectors for the case $\lambda = 0.005$ in the basis defined by the eigenvectors of the undeformed Hamiltonian. The levels with the smallest slope have a dominant component. It is the state with quantum numbers $n_y = 0$ and $n_x = N_{\text{shell}}$. Here, $N_{\text{shell}}$ denotes the shell number. The modulus of the amplitude of this component is 0.85 or larger and remains virtually unchanged for $\beta \leq 0.2$. Admixtures of non-dominant components with amplitude moduli greater than 0.1 are limited to a small number of states (ten or less). In contradistinction, the eigenvectors of the steepest levels are genuine mixtures without domi-
inant components. For $\beta > 0.1$, the number of essential components (amplitude moduli larger than 0.1) may be close to one hundred. There is a gradual transition, of course, from the levels with the smallest to those with the largest slope.

The wave functions of the dominant components correspond classically to orbits which oscillate in the $x$-direction, with little or no motion in the $y$-direction. The relative stability of these orbits is reflected in the small amount of mixing of their quantum analogues. We expect the bulk of the current to be carried by such orbits. The experimental set-up appears to enforce occupation of the associated characteristic levels as the conducting agent; otherwise a current could barely flow.

FIG. 4. Sections of the confining potential in (a) the $x$-direction and (b) the $y$-direction in a plane parallel to the surface at a distance of 0.01 $\mu$m. The rods on the surface are arranged as shown in the inset. The distance from top to bottom rod is 2 $\mu$m, the drawing is in scale. The three curves in (a) and (b) refer to a plunger potential (middle left rod) of $-V_0$, $-0.9V_0$ and $-0.85V_0$, respectively, where $-V_0$ is the potential at the other rods.

(ii) Is it reasonable to discuss deformation, and how does variation of the plunger gate voltage translate into a change of $\beta$? A quantitative answer would require precise knowledge of a particular experimental set-up, and we must confine ourselves to semiquantitative considerations. We consider a set of gates arranged as indicated in the inset of Fig. 4b. The current flows in the vertical direction. The middle left conducting rod serves as plunger gate. To study the potential well $V(x, y)$ formed beneath the gates, we have taken a set of line charges. This avoids solving the full boundary-value problem. The charges on the top, middle right and bottom rods were all chosen equal. Upon changing the charge on the plunger, they were re-adjusted to ensure that the potential values at the height of the entrance and exit barriers and at the tip of the middle right rod remain unchanged. An increase of the plunger voltage (charge) by 20% results in a decrease of 5% and 0.7% at the left hand and the right hand rods, respectively. Sections of the potential well confining the electrons taken in a plane below the gates are shown in Fig. 4, together with the changes due to an increase of the plunger voltage. In the $x$-direction, the bottom of the potential is lowered. In the $y$-direction, the same lowering is accompanied by a widening toward the left of the potential. Figure 4 indicates clearly the importance of deformation.

To describe these changes quantitatively, we approximate the potential by a paraboloid. The lowering of the bottom results in an effective increase of $\omega_x$. In the $y$-direction, there is an effective decrease of $\omega_y$. To first order in $\alpha$, we quantify these changes as $\omega_x \to (1 + \alpha)\omega_x$ and $\omega_y \to (1 - \alpha)\omega_y$. Rescaling the energy by a factor $(1 + \alpha)$ and writing $\beta = 2\alpha$, we obtain $\omega_y \to (1 - \beta)\omega_y$ while $\omega_x$ is fixed. This is the situation discussed above. With $-V_0 < 0$ the original value of the voltage on all the gates, an increase of the plunger potential from $-V_0$ to $-0.75V_0$ (a realistic range of values) causes, in the example in Fig. 4, a deformation $\beta \approx 0.1$. This is a sizeable value and corresponds to the scales shown in Figs. 1 and 3.

To relate $g_\beta\delta\beta$ and $g_{p_e}$, we estimate the change of depth of the harmonic oscillator potential needed to pull another electron into the dot. As shown in Fig. 4a, we require that the values of $V(\pm x_0, 0)$ remain unchanged under changes of the plunger voltage. Here, $\pm x_0$ denote the $x$-values of the positions of the barriers which define entrance and exit of the dot. We take $V(\pm x_0, 0) = E_F$. (Since there are barriers, the value of $E_F$ is actually slightly lower, but this is immaterial for what follows). In the case of Coulomb blockade without deformation [3], addition of one electron requires the potential to be lowered by $\Delta_x + e^2/C \approx e^2/C$. Here, $\Delta_x$ is the average single-particle level spacing and $e^2/C$ the charging energy. For $N$ electrons, this yields $Ne^2/C$. Measured from the points $\pm x_0$, the parabolic potential in $x$-direction must therefore have the depth $(1 + \alpha)^2(\omega_x x_0)^2/2 \approx E_F + Ne^2/C$. Inclusion of deformation modifies the value of $C$ but does not affect this argument qualitatively. We combine this result with the corresponding expression for the case of $N + 1$ electrons at deformation $\alpha + 1/2\delta\beta$ to obtain $\delta\beta \sim 2(e^2/C)/(\omega_x x_0)^2 \sim 1/N$. In the last step we have neglected $E_F$ in comparison with $Ne^2/C$. We compare this result with the average distance in $\beta$ of nearest avoided crossings. We consider the number $L$ of cross-
ings on a horizontal level at $N_{\text{shell}}$ in Fig. 1. We find that $L$ is governed by $[\beta/(1 - \beta)]N_{\text{shell}}^2/2$. For the distance of crossings this yields $\delta \beta \sim 1/N_{\text{shell}}^2 \sim 1/N$. This result is generic. The estimates show that roughly one level crossing occurs for each additional electron pulled into the dot. This result lends strong credibility to our model.

(iii) Figs. 1 to 3 represent the single-particle energies without taking account of the charging energy $U_0 = \epsilon^2/C$. To redress this omission, we use the framework of the self-consistent treatment of the Coulomb interaction within the quantum dot as applied in Ref. [11]. In the ordinary mechanism of avoided crossings, two levels $\epsilon_j(V)$ with $j = 1, 2$ are functions of an external parameter $V$. Let the two levels be coupled by a (real) matrix element $W$. The eigenvalues are

$$E_{\pm} = \frac{\epsilon_1 + \epsilon_2}{2} \pm \sqrt{\left(\frac{\epsilon_1 - \epsilon_2}{2}\right)^2 + W^2}. \quad (2)$$

If the two levels $\epsilon_j(V)$ intersect at some value $V = V_0$, then the eigenvalues $E_{\pm}$ show an avoided crossing at $V = V_0$. We now include the charging energy by considering two “effective” single-particle levels $\mathcal{E}_{\pm}$ defined as solutions of the mean-field equations $\mathcal{E}_{\pm} = E_{\pm} + U_0 \langle n_{\mp}\rangle$. Here the $\langle n_{\pm}\rangle$ are determined self-consistently,

$$\langle n_{\pm}\rangle = \frac{1}{\pi} \left[ \arctan \left( \frac{2(E_F - \mathcal{E}_{\pm})}{\Gamma_{\pm}} \right) + \frac{\pi}{2} \right], \quad (3)$$

where $\Gamma_{\pm}$ are the intrinsic widths of the two levels. We solve these equations self-consistently for $\mathcal{E}_{\pm}$ and $\langle n_{\pm}\rangle$ and pick the solution that minimizes the mean-field energy $E_{MF} = \langle n_{+}\rangle \mathcal{E}_{+} + \langle n_{-}\rangle \mathcal{E}_{-} - q\langle n_{+}\rangle \langle n_{-}\rangle$. We focus on a situation where the two effective levels are within an interval $U_0$ around the Fermi energy, with one level below $E_F$ and the other above it. As a result of the charging energy, the two levels participating in the avoided crossing are simply shifted apart by roughly $U_0$. The wave function at $V \ll V_0$ of the lower (higher) state is the same as the wave function at $V \gg V_0$ of the higher (lower) state. The mixing of the two wave functions near the avoided crossing is independent of the charging energy $U_0$. As a result, the wave function of the state that is occupied for $V \ll V_0$ changes smoothly into the wave function of the state which is empty, and available for the next electron, for $V \gg V_0$. This is in keeping with the mechanism proposed above.

Clearly, strong correlations must be expected for the conductance peak heights and for the transmission phases within a sequence of resonances caused by one and the same quantum state. Long sequences of this type are more likely to occur in quantum dots with regular shape. This might explain why long sequences of similar resonances where observed for the symmetric (regular) dot of Ref. [4] and perhaps weaker correlations in the more irregular dot of Ref. [3]. Our results suggest that further correlations not tested so far in Ref. [4] might exist. This possibility as well as a study of the effects of an applied magnetic field will be investigated in a forthcoming paper.

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