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# Coulomb oscillation amplitudes and semiconductor quantum-dot self-consistent level structure

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We calculate conductance versus gate voltage for single-electron tunneling through a lateral semiconductor quantum dot in the Coulomb blockade regime using the calculated self-consistent electronic structure of the device. We show that variations in the level spacings result in an experimentally observed but previously unexplained envelope modulation of peak amplitudes. We present a formula for the activated component of peak conductance as a function of level spacings and tunneling coefficients.

Capacitive lifting of the Coulomb blockade for tunneling in the linear source-drain bias regime through a lateral quantum dot defined electrostatically on a GaAs-$Al_xGa_{1-x}As$ two-dimensional electron-gas (2DEG) heterostructure, achieved via a metal gate positioned near the dot, results in a series of nearly equally spaced resonances of varying heights.[1-3] Though many of the features of these "Coulomb oscillations," notably the periodicity, are accounted for by the semiclassical theory which parametrizes the charging energy $U(N)$, for $N$ electrons in the dot, in terms of the device self-capacity and gate to dot capacitance and which is valid when the temperature $T$ is much greater than dot level broadening due to interaction with the leads;[4-6] nevertheless, a striking structure in the oscillation amplitudes has gone unexplained. Furthermore, the semiclassical calculation requires a set of dot energy levels $\varepsilon_p^0$, which must be assumed to be independent of $N$. Heretofore no attempt has been made to use realistic levels even for this "noninteracting spectrum"; rather, a single constant level spacing is usually assumed.

In this paper we present calculations of the self-consistent electronic structure for a lateral GaAs-$Al_xGa_{1-x}As$ quantum dot with $N\sim 70$. This is a factor of 5 larger than any results that we are aware of published to date[7] and is made possible by our procedure for decoupling the planar and transverse parts of Schrödinger's equation. Further, we derive a formula for and calculate the dot-contact-gate free energy from these self-consistent results. We thereby are able to compute the linear response conductance of the device with realistic $N$-dependent energy levels, $\varepsilon_p(N)$, and without employing capacitance parameters. As in the semiclassical calculations, the elastic couplings of the dot states to the source (drain), $\Gamma_p^{s(d)}$, remain as free parameters.

The principal result which we emphasize in this paper is that multioscillation, "envelope" modulation of the oscillation amplitudes, which has frequently been observed, results from thermally activated conductance through excited states of the dot combined with variations in the level spacings and/or tunneling coefficients.[8] Further, in contrast to an infinite 2DEG, the density of states (DOS) in a dot is a highly inhomogeneous, rapidly increasing function of energy. Consequently, the number of accessible *total dot states* (for fixed $N$) increases rapidly with $T$. Numerically we find that, for a dot at the small size limit of currently fabricated structures, Coulomb oscillation envelope modulation *from the DOS inhomogeneity alone* is observable for $T$ down to 50 mK.

Our model, in the Hartree approximation, of a semiconductor quantum-dot device similar in proportions but about 50% smaller than that devised by Kouwenhoven *et al.*[2] is schematically illustrated in Fig. 1(a). The calculation, which we will describe in more detail elsewhere,[9] is similar to those in the literature.[7] However, in order to solve Schrödinger's equation in the dot region for large $N$, rather than solving on a three-dimensional mesh as in Ref. 7, we compute an effective two-dimensional potential by first solving (at each iteration) the $z$-dependent Schrödinger equation at each point in the 2D plane. The resulting multicomponent 2D equation is then diagonalized in a suitable basis (typically Bessel functions). Poisson's equation must be solved on the full 3D mesh, but we simplify the $z$ dependence of the dot electron density to a constant across a 200 Å width. We fix $N$ and compute the chemical potential and the planar density by filling states according to a *Fermi* distribution [see discussion below Eq. (1)] of typically 0.5 K. Each level is treated as spin degenerate.

For a given $\{N, V_i\}$, where $V_i$ are the voltages applied to the gates [Fig. 1(a)], we calculate the total free energy of the dot-contact-gate system as follows. In its most general form the total *electrostatic* energy for the system can be written $W=\frac{1}{2}\int d\mathbf{r}\,\rho(\mathbf{r})\phi(\mathbf{r})$, where $\rho(\mathbf{r})=\rho_{\rm el}(\mathbf{r})+\rho_{\rm ion}(\mathbf{r})+\rho_{\rm ext}(\mathbf{r})$ is the sum of dot electron, donor ion, and contact-gate charge densities, respectively. For $\rho_{\rm ion}$ and $\rho_{\rm el}$, $\phi(\mathbf{r})$ is taken as the self-consistently computed potential, $\phi_{\rm sc}(\mathbf{r})$. For induced charges on gate (or contact) $i$, $\phi(\mathbf{r})=V_i$. We sum the dot electron energies and compensate for the double counting of the electron-electron interaction. The *free* energy must also account for the work done by the power supplies to charge the contacts, whereby we obtain

$$F(\{n_p\},N,V_i)=\sum_p n_p\varepsilon_p-\tfrac{1}{2}\int d\mathbf{r}\,\rho_{\rm el}(\mathbf{r})\phi_{\rm sc}(\mathbf{r})+\tfrac{1}{2}\int d\mathbf{r}\,\rho_{\rm ion}(\mathbf{r})\phi_{\rm sc}(\mathbf{r})-\tfrac{1}{2}\sum_i Q_iV_i\ , \qquad (1)$$

where $\{n_p\}$ specifies the occupancies of the dot levels, $Q_i$

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is the induced charge on gate (or contact) $i$, and $\rho_{el}$, $\phi_{sc}$, $Q_i$, and $\varepsilon_p$ depend implicitly on $\{N, V_i\}$.

We assume in Eq. (1) and below, where we calculate the temperature-dependent conductance, that small (thermal) variations in the level occupancies negligibly affect the self-consistent structure terms ($\varepsilon_p$, $\phi_{sc}$, $\rho_{el}$, and $Q_i$). This is well known for self-consistent studies of heterostructures[10] and, since our temperature range does not exceed a few K it is physically reasonable here. We find empirically that performing the electronic structure calculation at various temperatures below 4 K causes, in particular, essentially no change in the level spacings.

In the low-temperature and source-drain bias limit, tunneling through a dot which initially contains $N_0$ electrons is allowed only at discrete voltages which satisfy

$$\Delta F_0 \equiv F_0(N_0+1, V_C) - F_0(N_0, V_C) - E_F = 0 , \qquad (2)$$

where $F_0(N, V_C)$ is by definition the free energy computed from Eq. (1) with $n_p = 1$ $\forall p \leq N$ and $=0$ otherwise. Here and below all gate voltages except $V_C$ are held fixed.

The conductance of the dot as a function of gate voltage can be obtained by modifying the semiclassical result[4,5] to the following:[11]

$$G(V_C) = \frac{e^2}{k_B T} \sum_{\{n_i\}} P_{eq}(\{n_i\}) \sum_p \delta_{n_p,0} \frac{\Gamma_p^s \Gamma_p^d}{\Gamma_p^s + \Gamma_p^d} f(F(\{n_i+p\}, N+1, V_C) - F(\{n_i\}, N, V_C) - E_F) , \qquad (3)$$

where the first sum is over dot level occupation configurations and the second is over dot levels. The equilibrium probability distribution $P_{eq}(\{n_i\})$ is given by the Gibbs distribution, $f$ is the Fermi function, $E_F$ is the Fermi energy of the source and drain, and $\Gamma_p^{s(d)}$ are the elastic couplings of level $p$ to source (drain). The notation $\{n_i+p\}$ denotes the set of occupancies $\{n_i\}$ with the $p$th level, previously empty by assumption, filled.

To summarize, we choose a set of device parameters [Fig. 1(a)] and, on a grid of $V_C$ and $N$ values solve self-consistently for $\varepsilon_p$, $Q_i$ (from the surface electric fields), $\rho_{el}(\mathbf{r})$, and $\phi_{sc}(\mathbf{r})$. We then solve Eq. (3) numerically, using Eq. (1) to compute $F(\{n_i\}, N, V_C)$.

Figure 1(b) shows $\phi_{sc}(\mathbf{r})$ at the 2DEG level for $N=50$ and $V_C = -0.49$ V. Screening of the donors across the dot center results in a potential which is roughly 2D flat bottomed parabolic. In the $V_C$-$N$ plane Eq. (2) is satisfied along the $T=0$ "resonance curve" (inset Fig. 2). The nonlinear dependence of $V_C$ on $N$ shows that for our small dot the change in area, and hence the change in dot to gate capacitance, is non-negligible.

The spectrum along the resonance curve is plotted in Fig. 2. Triangles mark the $N$th or "quasi-Fermi" level, $E_F^*$. All depicted levels are in the lowest $z$ subband, whose energy is $\approx 2$ Ry*. Below $N=58$ ($V_C \lesssim -0.4$ V) the levels tend toward the degeneracies characteristic of a bare 2D parabolic potential (1,2,3,. . .). More negative gate voltages ($V_C \lesssim -0.55$ V) distort the dot and lift the degeneracy of the higher states. At higher $N$ the electrons screen the parabolic potential and the spectrum reflects the flatness at the center. The precise form of the spectrum will be affected by a realistic $z$ dependence of the wave functions and charge distribution, by details of the donor configuration and by exchange-correlation effects,[12] all of which we have neglected. Note, however, that although gate $C$ [Fig. 1(a)] asymmetrically biases the dot, the levels change smoothly and no "chaotic" variation, as discussed by Jalabert, Stone, and Alhassid,[13] is observable. We believe that the assumption which those authors make of a flat-bottomed, infinite hard-wall potential produces anomalous sensitivity to small variations in confining shape.

The conductance as a function of gate voltage corresponding to the spectrum in Fig. 2 is shown in Fig. 3 for $T=0.25$ K ($k_B T \approx 0.004$ Ry*). For comparison with the level spacings in Fig. 2 we have set all the tunnel coefficients to unity. The envelope structure of the oscil-

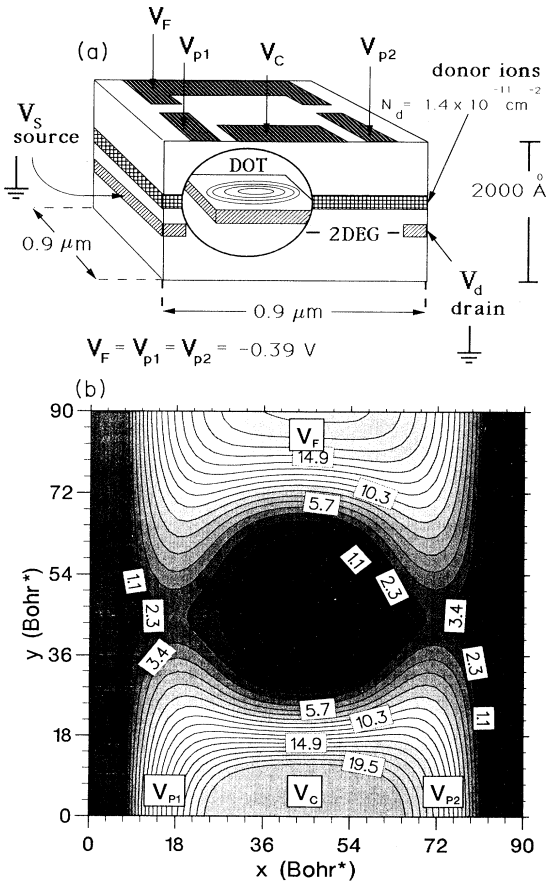


FIG. 1. (a) Quantum-dot single electron tunneling device model showing surface gate configuration and parameters used in these calculations. (b) Self-consistent electrostatic potential contour for $N=50$ and $V_C = -0.49$ V at the 2DEG level. Contours are in Ry*. Surface gate positions (1200 Å above the 2DEG level) are labeled.

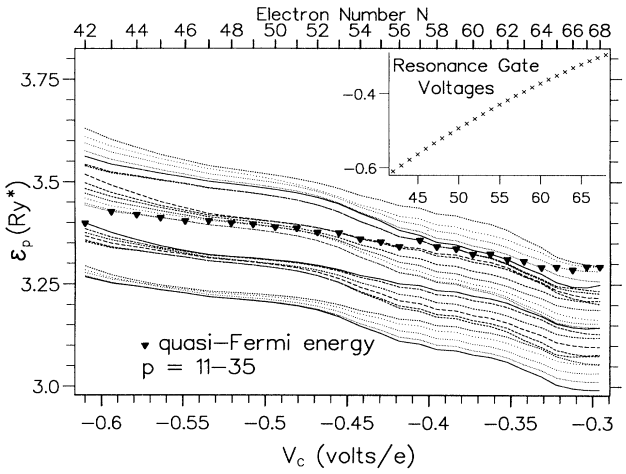


FIG. 2. Effective single electron energy levels measured with respect to the dot potential minimum for (spin-degenerate) states $p=11-35$, as a function of $V_C$. Electron number $N$ also varies along the curves so that Eq. (2) is always satisfied. Lines between integer $N$ points are guides to the eye. All states are ground $z$ subband and include that energy of $\approx 2$ Ry*. Triangles mark the $N$th or "quasi-Fermi" level. Inset is plot of $V_C$ (in V), $N$ points at which Eq. (2) is satisfied.

lations in Fig. 3 follows the variation in level spacing at the Fermi surface in the spectrum of Fig. 2. By calculating this characteristic at increasing temperatures we find that the enhanced (i.e., above $e^2/h$) peak conductances all increase exponentially (cf. Fig. 4). We may analytically estimate the expected enhancement and its dependence on level spacings near the Fermi surface as follows. Near the $N_0$th resonance the $T\to 0$ limiting form of Eq. (3) is (cf. Ref. 14)

$$G^0(V_C,T)=\frac{e^2}{k_BT}\frac{\Gamma_{N_0+1}}{3+a_1e^{\beta\Delta F_0}+a_2e^{-\beta\Delta F_0}}, \tag{4}$$

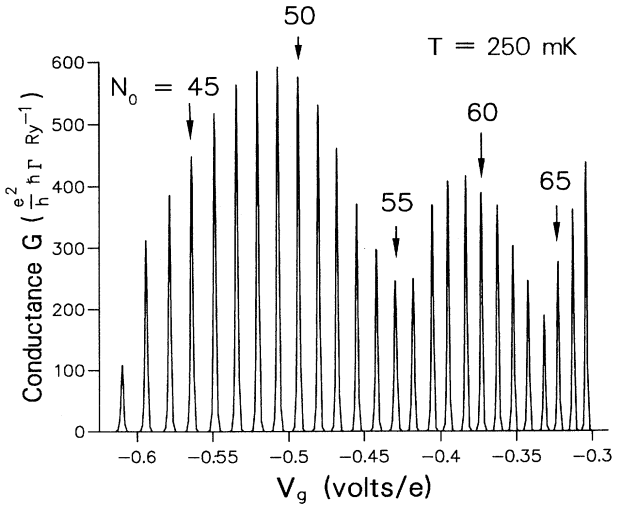


FIG. 3. Conductance as a function of gate voltage for parameters in Fig. 1(a) and levels in Fig. 2. If conductance value is multiplied by dot level width, $\hbar\Gamma$ in Ry*, resulting value is in units of $e^2/h$.

where $\beta\equiv 1/k_BT$, $(a_1,a_2)=(2,1)$ for $N_0$ odd and $=(1,2)$ for $N_0$ even and where we have assumed $\Gamma_p^s=\Gamma_p^d$. Writing $\Delta F_0=A(V_C-V_C^0)$, where $V_C^0$ is the zero-temperature resonance position and $A$ is a constant, for finite temperature the position of the maximum in Eq. (4) is given by $V_C^{\rm res}=V_C^0+(k_BT/A)\ln(a_2/a_1)$. This resonance *position* is to lowest order unaffected by tunneling through excited dot states, hence we can enumerate terms in Eq. (3) to find the next contributions to $G(V_C^{\rm res},T)$. The analysis, which is tedious but straightforward, is simplified if we assume that the level *spacings* (cf. Fig. 2), $\Delta^p(N,V_C)\equiv\varepsilon_p(N,V_C)-\varepsilon_{p-1}(N,V_C)$, change negligibly as a single electron is added to the dot. Defining the (dimensionless) activated conductance as $g(V_C^{\rm res},T)\equiv(k_BT/\hbar\Gamma_{N_0+1})[G(V_C^{\rm res},T)-G^0(V_0^{\rm res},T)]/(e^2/h)$ we find for the lowest-order contributions of the two levels closest to the quasi-Fermi surface

$$g(V_C^{\rm res},T)/2\pi=e^{-\beta\Delta^{N_0+1}}[b_1(\Gamma_{N_0-1}/\Gamma_{N_0+1})-b_2]+e^{-\beta\Delta^{N_0+3}}[b_3(\Gamma_{N_0+3}/\Gamma_{N_0+1})-b_4] \tag{5}$$

for $N_0$ even; where $b_1=2/(1+\sqrt{2})$, $b_2=\sqrt{2}/(3+2\sqrt{2})^2$, $b_3=1/(2+\sqrt{2})$, and $b_4=(2+\sqrt{2})/(3+2\sqrt{2})^2$. (For $N_0$ odd, replace $N_0$ by $N_0-1$ everywhere and interchange $b_1,b_2$ with $b_3,b_4$, respectively.) We can compute the activated conductance from the full numerical solution of

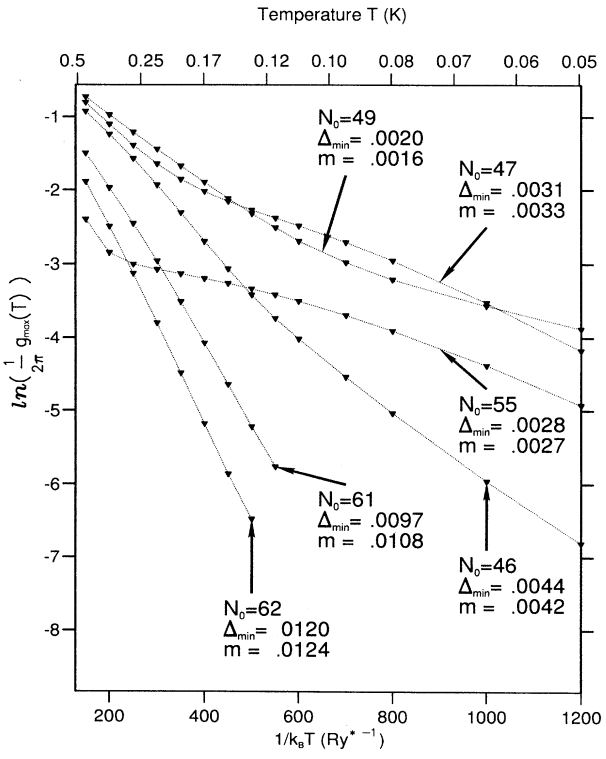


FIG. 4. Logarithm of activated conductance for various resonances in Fig. 3 as a function of $\beta=1/k_BT$. Low-$T$ asymptotic slopes $m$, and smallest level spacing $\Delta^{\rm min}$ in Ry*, for each resonance are listed.

Eq. (3) and compare with the behavior expected from Eq. (5) with the appropriate level spacings (Fig. 2) inserted. (Again, the $\Gamma$'s are set to unity.) For sufficiently low temperature, we have from Eq. (5) that $(\partial/\partial\beta)\ln[g(V_C^{\rm res},T)/2\pi]\rightarrow-\Delta^{\rm min}$ where $\Delta^{\rm min}$ is the smaller of the two level spacings in Eq. (5). Thus in Fig. 4 we plot $\ln[g(V_C^{\rm res},T)/2\pi]$ [this is computed from the full numerical solution of Eq. (3) at a variety of temperatures] versus $\beta$ for a variety of the resonances in Fig. 3. The low-temperature limiting values of the slopes of each curve, along with the values of $\Delta^{\rm min}$ from the level spacings, are noted. Note that where the level spacing is large (in particular $N_0=62$ and 61), activated conductance from all but the nearest level quenches at relatively high temperatures.

Approximate symmetries (e.g., azimuthal) in the confining potential and the "soft" walls of the dot lead to a highly nonuniform energy spectrum with levels becoming overall more closely spaced with increasing energy (Fig. 2). This bunching of levels tends to lower the temperature of the regime where oscillation amplitudes represent only an individual $\Gamma_p$. Further, while activated tunneling is suppressed by the Boltzmann factors in Eq. (5), the combinatorial prefactors $b_i$ reflect the rapid increase with thermal energy in the number of accessible *total dot states* and hence conducting channels. Our calculations show that even for this small dot some oscillations possess a significant activated component down to 50 mK (Fig. 4).

While our numerical conductance results focus on the influence of level spacing on the resonance amplitudes, both varying level spacings and varying tunnel coefficients, through the correlating effect of thermal activation, impart an envelope modulation to the oscillations.[8] From any prescribed set of level spacings and tunneling coefficients, $\{\Delta^p,\Gamma_p\}$ Eqs. (4) and(5) can be used to compute the "turn on" of activated conductance as the temperature is raised. Conversely, a detailed study of the temperature dependence of a consecutive series of oscillations can be fit with Eqs. (4) and (5) to *deduce* both the $\Gamma_p$'s and the $\Delta^p$'s. Though temperature dependence of individual oscillations has been published,[1] we propose that this experiment, by examining the correlated temperature dependence of a series of resonances, will uncover a wealth of information on quantum-dot electronic structure which can be compared with that from other probes, such as nonlinear transport measurements.[15] Quite possibly the necessary data have already been accumulated although, in the absence of a simple expression relating amplitudes to level spacings and tunnel coefficients, they have not been fully analyzed.

In conclusion, we have computed the self-consistent spectrum for a lateral semiconductor quantum dot for electron number of order 70. We have derived a formula for the interacting dot/contact/gate system free energy in terms of the electronic structure results. We have computed the linear response conductance through the dot and shown that level spacing and combinatorial factors produce a larger than expected thermally activated component of the current. We have demonstrated that experimentally observed correlation and envelope modulation of peak amplitudes is a thermal effect resulting from variations in the level spacings and/or tunneling coefficients. We derive a formula for peak amplitude temperature dependence which can be compared directly with experiment to independently determine the Fermi surface level spacings and tunneling coefficients.

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