Many-body effects in resonant tunneling through quantum dots

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We show that the resonance energies associated with tunneling through a typical semiconductor dot depend strongly on quantum-mechanical many-body effects in the dot. These resonance energies *cannot* be written as the sum of single-particle confinement energies and constant Coulomb charging energies, and the magnetic-field dependence of these resonance energies differs greatly from the single-electron result. The semiclassical description of Coulomb charging effects in terms of capacitances is shown to be incorrect.

Recent measurements of transport through zero-dimensional semiconductor structures (quantum dots) have yielded current-voltage data with rich structure.[1-5] The interpretation of such data is difficult since there are many comparable energy scales in the problem, and the quantum dot contains a varying number of electrons when carrying a current. Typically the electron-electron interaction between electrons in the dot, the single-electron confinement energy, and the cyclotron energy are all on the meV scale, and hence all these effects must be included in a quantum-mechanical, many-electron description of the system. Earlier work on larger dots probed the regime where the confinement energy is much smaller than the electrostatic energy.[6] However, attention has recently turned to the regime in which energy quantization and charging effects in the dot are of equal importance.[1-3] In attempting to interpret such data,[1-3] it is often assumed that the resonance energies can be described by the sum of single-particle confinement energies and constant Coulomb charging energies. More sophisticated theories have included Hubbard-like terms to describe the electron-electron interaction in the dot.[7,8] Such constant Coulomb terms do not, however, take into account the dependence of the Coulomb repulsion on the separation of electrons in the dot. In this paper, we use exact results from an analytically solvable model of interacting electrons in a quantum dot[9,10] to show the following for a typical semiconductor dot: (i) the quantum-mechanical many-body effects dramatically alter the resonant tunneling energies; (ii) the magnetic-field dependence of these resonance energies differs significantly from the single-electron result; (iii) the resonance energies of the dot *cannot* be written as the sum of single-particle confinement energies and constant, magnetic field-independent, Coulomb charging energies; (iv) the semiclassical description of Coulomb charging effects (e.g., Coulomb blockade, Coulomb staircase[6]) in terms of capacitances is incorrect.

We consider a quantum dot coupled to leads on each side. The dot will act as a scattering center for electrons and the quasibound states (resonances) of the dot are expected to give rise to features in the current-voltage characteristic. Our model Hamiltonian for an isolated, quasi-two-dimensional[1-5] quantum dot in a perpendicular magnetic field B is[9]

$$H=\frac{1}{2m^*}\sum_i\left[\mathbf{p}_i+\frac{e\,\mathbf{A}_i}{c}\right]^2+\tfrac{1}{2}m^*\omega_0^2\sum_i|\mathbf{r}_i|^2+\sum_{i<j}V(\mathbf{r}_i,\mathbf{r}_j)-g^*\mu_B B\sum_i S_{i,z}\ . \tag{1}$$

The parabolic dot lies in the x-y plane and contains N interacting electrons with effective mass m^*, negative charge $-e$, effective g factor g^*, spatial coordinates $\mathbf{r}_i=(x_i,y_i)$, and spin components $s_{i,z}$ along the z axis. The quantity $\mathbf{A}_i$ is the vector potential and μ_B is the Bohr magneton. The interaction potential is given by

$$V(\mathbf{r}_i,\mathbf{r}_j)=2V_0-\tfrac{1}{2}m^*\Omega^2|\mathbf{r}_i-\mathbf{r}_j|^2\ , \tag{2}$$

where V_0 and Ω are positive parameters. The saturation of $V(\mathbf{r}_i,\mathbf{r}_j)$ for small electron separations models the effect of the finite electron wave function spread along the perpendicular (z) direction. With $V_0=10$ meV and $\hbar\Omega=5.6$ meV, the model interaction shows similar behavior to a cutoff Coulomb interaction[11] for separations between 0 and 350 Å; the upper limit is of the order of the electron-gas diameter in a typical GaAs dot with $\hbar\omega_0=15$ meV.[9,10] Different values of V_0 and Ω will model dots of different sizes.

In order to tunnel through a dot that initially contains N electrons, an electron in the emitter lead needs enough energy to leave the lead and enter the dot, which then becomes an $(N+1)$-electron system. In this paper, we concentrate on the energy required to increase the number of electrons in the dot although we will briefly describe the effect of interaction between the dot and the leads and other nearby conductors. Hence we first consider the leads to be at infinity so that any rearrangement of the electrons in them during the tunneling process has negli-

gible effect on the energy levels of the dot (i.e., the dot is isolated). Suppose the dot initially contains N electrons ($N=0,1,2,\ldots,$) in a particular eigenstate $|N;i\rangle$ of H with corresponding eigenvalue $E(N;i)$. Consider an $(N+1)$-th electron in the emitter lead with energy E_0. Neglecting tunneling through virtual states, the $(N+1)$-th electron in the emitter can tunnel into the dot when $E_0=E(N+1;j)-E(N,i)$, where $E(N+1;j)$ is an eigenvalue corresponding to state $|N+1;j\rangle$ of the quantum dot with $N+1$ electrons. [For noninteracting electrons, $E(N+1;j)$ can be written in the form $E(N;i)+\varepsilon(j)$ where $\varepsilon(j)$ is a single-particle energy of the quantum dot. Hence $E_0=\varepsilon(j)$ and the resonant tunneling peaks occur at the single-particle levels of the quantum dot as expected.] In general, there are a multitude of excited states $|N+1;j\rangle$, and many possible decay processes for the excited $(N+1)$-electron dot system.

Here we focus on one particularly important tunneling channel where the exact dot eigenstates $|N;i\rangle$ and $|N+1;j\rangle$ have the additional property of being the *ground* states for large magnetic field, the regime probed experimentally in Ref. 1. Similar conclusions can also be obtained from considering other tunneling channels. For convenience we label these particular eigenstates $|N;i\rangle$ and $|N+1;j\rangle$ as $\Psi_0(N)$ and $\Psi_0(N+1)$. We shall briefly describe the variation of the energy of state $\Psi_0(N)$. The overall spin state of Ψ_0 is symmetric since the electron spins are aligned parallel to the field. The corresponding spatial state of $\Psi_0(N)$ is antisymmetric and has a wave function

$$\prod_{i<j}(x_{ij}-iy_{ij})\exp\left[-\frac{Nm^*\omega_0(B)}{2\hbar}(X^2+Y^2)\right]\times\exp\left[-\frac{m^*\Omega_0}{2N\hbar}\sum_{i<j}(x_{ij}^2+y_{ij}^2)\right],$$

where $\omega_0^2(B)=\omega_0^2+\omega_c^2/4$, $\Omega_0^2=\omega_0^2(B)-N\Omega^2$; $\omega_c=eB/m^*c$, $\mathbf{r}_{ij}=(x_{ij},y_{ij})=\mathbf{r}_i-\mathbf{r}_j$, and $\mathbf{R}=(X,Y)=(1/N)\sum_i\mathbf{r}_i$. The energy of the state $\Psi_0(N)$ is given by

$$E(N)=\hbar[\omega_0(B)+\tfrac{1}{2}(N-1)(N+2)\Omega_0-\tfrac{1}{4}N(N-1+4\alpha)\omega_c]+N(N-1)V_0 \quad (3)$$

with $\alpha=g^*m^*/4m_0$. Curve A in Fig. 1 shows the total energy $E(N)$ of state $\Psi_0(N)$ as a function of magnetic field ($\hbar\omega_c$) for $N=5$ interacting electrons in a GaAs dot with $\hbar\omega_0=15$ meV. The behavior of $E(N)$ can be understood from the limiting cases shown by curves B–D in Fig. 1. In the absence of the electron-electron interaction, $E(N)$ becomes a sum over single-particle energies, and is given by (curve B)

$$E_B(N)=\frac{\hbar}{2}[N(N+1)\omega_0(B)-\tfrac{1}{2}N(N-1+4\alpha)\omega_c]\ . \quad (4)$$

In the absence of the Pauli exclusion principle, but retaining the electron-electron interaction, $E(N)$ becomes (curve C)

$$E_c(N)=\hbar[\omega_0(B)+(N-1)\Omega_0-\alpha N\omega_c]+N(N-1)V_0\ . \quad (5)$$

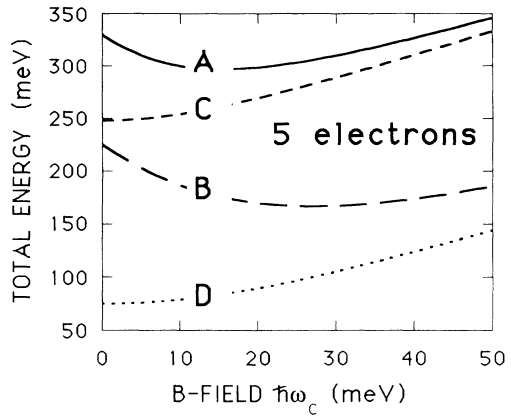

FIG. 1. Total energy $E(N)$ (curve A) of $N=5$ electrons in a GaAs dot ($\hbar\omega_0=15$ meV) in eigenstate $\Psi_0(N)$, as a function of magnetic field. Curves B, C, and D correspond to the energies $E_B(N)$, $E_C(N)$, and $E_D(N)$ defined by Eqs. (4)–(6), respectively.

In the absence of both the Pauli exclusion principle and the electron-electron interaction, $E(N)$ becomes (curve D)

$$E_D(N)=N\hbar[\omega_0(B)-\alpha\omega_c] \quad (6)$$

which is obviously just five times the single-particle energy. Both $E_D(N)$ and $E_C(N)$ increase with B field due to increasing kinetic energy (wave-function shrinkage). The zero-field value of $E_B(N)$ is lower than that of $E_C(N)$ since the kinetic-energy cost due to the Pauli exclusion principle is smaller than the electrostatic potential energy. The energies $E(N)$ (curve A) and $E_B(N)$ tend to the values of $E_C(N)$ and $E_D(N)$, respectively, at large fields, since in this limit the fermion statistics of the particles becomes less important. The potential energy due to the electron-electron interaction, $E(N)-E_B(N)$, increases by 50% from 105 meV at $\hbar\omega_c=0$ to 160 meV at $\hbar\omega_c=50$ meV as a result of the reduction in the typical electron-electron separation with increasing $\hbar\omega_c$. Therefore the total dot energy $E(N)$ cannot be written as a sum of single-particle energies [i.e., $E_B(N)$] plus a constant Coulomb charging energy. If we try to interpret a capacitance for the isolated dot ($C_{\rm dot}$) by setting $E(N)-E_B(N)$ equal to the classical charging energy $(Ne)^2/2C_{\rm dot}$, we obtain $C_{\rm dot}=(Ne)^2/\{2[E(N)-E_B(N)]\}$ which is a complicated function of N and $\hbar\omega_c$, and does not correspond to a classical capacitance.

Curve A in Fig. 2 shows the resonant tunneling energy $\Delta(N)$, defined as $E(N+1)-E(N)$ minus the spin-up energy of the $(N+1)$-th electron, through a dot initially containing $N=5$ electrons. The energy $\Delta(N)$ is given by

$$\Delta(N)=\frac{\hbar}{2}[N(N+3)(\Omega_0^2-\Omega^2)^{1/2}-(N-1)(N+2)\Omega_0-N\omega_c]+2NV_0\ . \quad (7)$$

In the absence of the electron-electron interaction, $\Delta(N)$ becomes (curve B)

$$\Delta_B(N)=\hbar[(N+1)\omega_0(B)-\tfrac{1}{2}N\omega_c]\ . \quad (8)$$

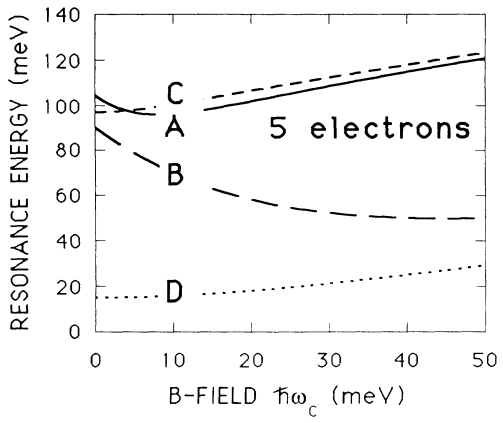

FIG. 2. Resonance energy $\Delta(N)$ (curve A) for an incident spin-up electron tunneling through a GaAs dot ($\hbar\omega_0=15$ meV) containing $N=5$ electrons, as a function of magnetic field. Curves B, C, and D correspond to the quantities $\Delta_B(N)$, $\Delta_C(N)$, and $\Delta_D(N)$ defined by Eqs. (8)–(10), respectively.

In the absence of the Pauli exclusion principle, but retaining the electron-electron interaction, $\Delta(N)$ becomes (curve C)

$$\Delta_c(N)=\hbar[N(\Omega_0^2-\Omega^2)^{1/2}-(N-1)\Omega_0]+2NV_0 \ . \quad (9)$$

In the absence of both the Pauli exclusion principle and the electron-electron interaction, $\Delta(N)$ becomes (curve D)

$$\Delta_D(N)=\hbar\omega_0(B) \ . \quad (10)$$

The energy contribution due to the electron-electron interaction $\Delta(N)-\Delta_B(N)$ increases by 400% from 14 meV at $\hbar\omega_c=0$ to 71 meV at $\hbar\omega_c=50$ meV. In addition $\Delta_B(N)$ decreases monotonically over this range while $\Delta(N)$ (curve A) shows an overall increase. Therefore the resonant tunneling energy $\Delta(N)$ cannot be written as a single-particle energy term [i.e., $\Delta_B(N)$] plus a constant Coulomb energy term.

In the special case when $\Omega \ll (\omega_o^2/N+\omega_c^2/4N)^{1/2}$, it follows from Eqs. (3), (4), (7), and (8) that $E(N) \approx E_B(N)+N(N-1)V_0$ and $\Delta(N)\approx\Delta_B(N)+2NV_0$. This separation into single-particle energies and Coulomb terms is now reasonable since, for small Ω, large ω_0 or large ω_c, the electron-electron interaction is nearly constant ($\approx 2V_0$) over the radius of the electron gas (cf. Hubbard model). In this limit, $C_{\rm dot}\approx(Ne)^2/[2N(N-1)V_0]$ which yields the constant value $e^2/2V_0$ for large N. Setting the Coulomb saturation energy $2V_0\sim e^2/a$, where a is the electron gas radius in the z direction, yields $C_{\rm dot}\sim a$ for large N, which is the result expected for a classical, spheroidal conductor. However we stress that the approximation $\Delta(N)\approx\Delta_B(N)+2NV_0$, which is that used in Ref. 1 ($2V_0=U$, where U is a constant Coulomb energy), is generally invalid.

We now give a qualitative discussion of the effects of nearby leads and gates. Quantitative details will depend upon specific device design, and are beyond the scope of this paper. To a first approximation, the total energy of the isolated dot $E(N)$ will decrease by $(Ne)^2/2C_{\rm eff}$ in the presence of nearby conductors, where $C_{\rm eff}$ reflects the change in capacitance of the isolated dot due to image charges induced in the conductors. The classical N^2 dependence reflects the fact that the negative charges on the dot are spatially separated from image charges in the leads, and hence in contrast to the isolated dot, there is no self-interaction term. The magnitude of the energy $(Ne)^2/2C_{\rm eff}$ has been estimated to be smaller than $E(N)$ for typical semiconductor dots.[3] However, as $E(N)$ does not have an N^2 dependence, even for the special case mentioned, the total dot energy is not proportional to N^2 and therefore cannot be described in terms of an effective total capacitance. The semiclassical description of Coulomb charging effects in terms of a total dot-lead capacitance is consequently incorrect. We note finally that the proximity of leads and gates can also introduce a complicated electric-field distribution at the dot, thus perturbing the N-electron wave functions and energies. However, a constant electric field merely shifts the origin of the wave functions of a parabolic potential, hence only the nonuniform contribution to the electric field over the region of the dot can actually cause changes to the energies that we have evaluated in this work.

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