Charging effects and increasing transparency in double-barrier structures

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(Received 31 October 1994)

We present a dynamical analysis of charge accumulation effects during tunneling in a double-barrier structure using a self-consistent treatment of the electron-electron interaction. Resonance peaks seen in typical transmission coefficient spectra for noninteracting electrons appear shifted to higher energies depending on the magnitude of the charge density in the well, as well as on the spatial dependence of the wave function describing the resonances. The total charge in the well exhibits a well-defined Coulomb staircase for the case of sharp resonances, and only a smoothly increasing behavior for more open systems.

The observation of periodic conductance oscillations in systems where electrons are confined in narrow channels or small quantum dots and partially isolated by potential barriers has stimulated the work of many authors.[1] Important experimental and theoretical efforts have been made to understand the properties and explore the potential applications of such systems.[2] The physical dimensions of these structures have reached levels such that their capacitance C can be as small as 10^{-16} F. One then has a situation where the Coulomb charging energy $e^2/2C$ ($\simeq$ 1 meV) is larger than the average single-electron energy level spacing $\Delta\epsilon$ ($\simeq$ 0.1 meV), and for sufficiently low temperatures one has $\Delta\epsilon > k_BT$. Under these conditions, it has been shown[3–5] that the interplay between Coulomb interaction and energy quantization plays a decisive role in the explanation of many observations. Spectroscopic studies of individual microstructures via electron transport,[6–9] and single-electron capacitance,[10] have been carried out with great success. Possible applications have also been suggested, through the development of "electron-turnstile,"[11] or "electron pump"[12] devices, where the potential barriers are manipulated to allow the passage of single electrons at a desired rate.

Different aspects of this problem have been studied theoretically using various techniques.[13–15] In a seminal paper, Meir *et al.*[13] used an equation of motion for the Green's function, to study the temperature dependence of the conduction peaks. Their work is based on an Anderson impurity model with the site coupled weakly to ideal noninteracting leads, the electronic interaction described by a Hubbard term, and the use of a generalized Landauer-type formula.[14]

More recently, Palacios *et al.*[16] have studied the conductance of such systems in a magnetic field using a Keldysh framework.[14] Nonlinear transport properties of quantum dots have been studied by Weinmann *et al.*[17] using a master equation approach for the time evolution of the occupation probabilities of many electron states. Also, Pfannkuche and Ulloa have explored the tunneling selection rules introduced by electronic correlations.[18] These approaches rely on the solution of an interacting system with hard/closed walls, which is then opened to the leads via small overlap matrix elements included within perturbation theory. Here, the coupling to the leads is typically considered *fixed*, rather than obtained after the self-consistent readjustment of the system to the additional charge and potentials. These approximations, although believed to be correct for long-lived and isolated resonances (in the so-called *Coulomb blockade* regime), are expected to break down for the case of more transparent walls or large bias voltages.

In this paper, we propose an intuitive dynamical approach to study charging effects on resonant tunneling in a double barrier structure, using a *self-consistently* determined potential to take into account electron-electron interactions in the well. We treat an *open* system and correspondingly study the transmission coefficient as a function of energy for the interacting system, using a tight-binding representation. In this fashion, both the coupling to the leads and the interaction effects are treated on a more equivalent footing, as the charge trapped within the well readjusts the effective potential and this in turn affects the transparency of the system. In particular, we find that the transmission coefficient exhibits resonances similar to the noninteracting single-electron case. As one would expect intuitively, these resonances are shifted upwards in energy but with a shift not given by a simple constant, as the classical charging model would predict.[4,5] In fact, the shift is closely related to the spatial extent and corresponding charge distribution of the specific resonant wave function. We further find that this shift slowly decreases for large resonance (or electron) numbers, as one would expect for a free-flowing Fermi quasiparticle, as the total accumulated charge continues to increase but only slowly for higher Fermi energies.

We should mention that a somewhat similar framework has been developed by Presilla *et al.*[19] to study the time evolution of the charge stored in a three-dimensional potential well and its effect on the transmitted and reflected fluxes.[20] Also, Orellana *et al.*[21] have studied possible bistability in the presence of a magnetic field, and Zhang

et al.[22] have studied the apparent plasmon-coupling signature seen in resonant-tunneling experiments. The method we present here is qualitatively similar to some of these, and is conceptually and numerically simpler than the Keldysh-derived calculations.[23]

In what follows, we describe our formalism and present a few characteristic results. We consider the problem of transmission of an electron incident with energy E on a region such as a quantum dot or a double-barrier structure, where electron-electron interactions are important. The leads are assumed to be well described by a quasiparticle Fermi gas, as the high level density there yields a much more effective screening than in the well.[13,14] [Notice that this approximation should be appropriate for the lateral transport experiments in quantum dots.[6–9] However, tunneling via two-dimensional (2D) accumulation layers in double-barrier heterostructures would give rise to other interesting effects, as discussed recently.[24]] This central region is limited by left and right potential barriers of height β_0 and β_L, respectively [see inset Fig. 1(b)].

Using a tight-binding approximation with lattice sites separated a distance a, we can expand the wave function of the system as $\Psi(x) = \sum_i c_i \phi_i(x)$, where $\phi_i(x)$ is a local orbital centered on site i, c_i is the probability amplitude for finding the electron on this site, and the sum is taken over all lattice sites. Substituting in the Hamiltonian, we obtain an equation for the coefficients c_i, given by

$$E\,c_i = E_0\,c_i - t\,c_{i-1} - t\,c_{i+1} + v_i\,c_i\,, \tag{1}$$

where E_0 is the on-site energy, t is the hopping integral, and the last term represents the Coulomb interaction. (We have made the usual tight-binding nearest-neighbor approximations. A continuum differential equation is also tractable, although it makes the numerical computation somewhat more involved.) We assume here that v_i is given by a site-Hubbard expression in the interacting region between the barriers, so that

$$v_i = U\rho_i\,, \qquad 1 \le i \le L-1\,, \tag{2}$$

$v_L = \beta_L$, and $v_0 = \beta_0$, and the distance between barriers is La (with L an integer). Here U is a parameter measuring the strength of the local interaction (and in experiments depends on the structural confinement, and potential gate screening effects, according to the specific system implementation). The electronic density at each site i is given by

$$\rho_i(E) = \int_0^E |c_i(E')|^2\, g(E')\, dE'\,, \tag{3}$$

where $g(E) \sim E^{-1/2}$ is the density of states in 1D. It is important to emphasize that the interaction term is a function of the incident energy E and has to be evaluated at each step of the calculation. Notice that for transport in the linear regime, the incident energy is the excess kinetic energy of the electrons from the reservoir, measured with respect to the *local well potential*, which is typically controlled in experiments via gates (and at zero bias is then the Fermi energy in the leads/reservoirs). This results in all levels below E to be occupied in equilibrium. In this approach, charging effects within the interaction region represent an additional potential at each site which inhibits further electron passage. This yields the expected Coulomb blockade effects whenever charge accumulates in the well and readjusts the energy level structure. On the other hand, in the region outside the barriers, the non-interacting-electron tight-binding dispersion relation remains valid, $E = E_0 - 2t\cos ka$, so that one can relate the incident energy with the propagation wave number outside the well k.[25]

For convenience, we measure all energies in units of $t = 1$ meV, and lengths in terms of $a = 200$ Å, in such a way that $L = 10$ corresponds to a typical experimental "device" in GaAs nanostructures (~ 0.2 μm). We then get $\Delta\epsilon \sim 0.1$ meV, for the average energy level spacing, similar to the values discussed in experiments. Equation (1) is solved for fixed β_0, β_L, and L values, with the interaction term v_i given by (2), and incorporating the information on energy level occupation via Eq. (3). For convenience of computation, we assume particles incident from the right at $x = La$, being transmitted to the left at $x = 0$. The transmission amplitude t_0 is fixed to unity, so that we calculate the incident amplitude i_0 [see inset Fig. 1(b)]. In this case, the transmission coefficient T is given by $T = 1/|i_0|^2$, and the following expression is obtained from the boundary conditions,[26]

$$T = \frac{|e^{2ika} - 1|^2}{|\tilde{c}_{L+1} - \tilde{c}_{L+2}e^{-ika}|^2}\,, \tag{4}$$

where the $\tilde{c}_i$ coefficients are then normalized to *unit transmission.*

The solution of Eq. (1) is carried out starting from initial values $\tilde{c}_0 = t_0 = 1$, and $\tilde{c}_{-1} = t_0 e^{ika}$, and after back substitution we obtain the remaining coefficients $\tilde{c}_i$ for each value of the energy. The transmission coefficient T is then calculated from Eq. (4), as well as the c_i coefficients (normalized to *unit incidence*), such that $|c_i(E)|^2 = T(E)|\tilde{c}_i(E)|^2$. The sharp E dependence of T and the integrand in (3) requires the use of adaptive integration techniques, but it is easily handled recursively.[27]

We should make some comments on the approximations. First, notice that Eqs. (1) to (3) can be generalized to include higher-order terms in the interaction, resulting in an "extended Hubbard model" with exchange and correlation terms (similar to a set of Kohn-Sham equations in the local density approximation).[28] Our main purpose here is to show that the approach is workable and yields sensible results. The possible inclusion of those terms and specific geometries would allow direct comparison with experiments.

Moreover, notice that an implicit assumption in our treatment is that one can allow the system to reach a steady-state configuration (since we iterate to self-consistency). This approximation gives the proper intuitive results and is believed to be correct, as long as one is not interested in time-dependent effects (where out-of-equilibrium transient configurations would be important), or where coherent coupling between the well

states and the leads is relevant (which would be the case at extremely low temperatures, where a Kondo-like resonance appears at the Fermi level).[29]

Figure 1(a) shows the effect of a small interaction constant ($U = 0.5$) on the transmission coefficient as a function of incident energy, for a case where the barrier heights are sufficiently large ($\beta_0 = \beta_L = 5$) so that the resonances are well isolated (especially those at low energies). It is clear that the resonances are shifted to higher energies and have larger widths than in the noninteracting case. The shift is accompanied (or produced) by the accumulation of charge in the well, as shown in Fig. 1(b). In fact, the total electron density in the well shown there, $\rho(E) = \sum_j \rho_j(E)$, increases in a nearly stepwise fashion in multiples of the elementary charge, whenever a new resonant state passes below the incident energy, and remains nearly constant until the next resonance. This picture of *sequential* charging of the well, as the local potential drops with respect to the external reservoir, is of course in agreement with the classical ideas of dot or well charging used to explain the Coulomb blockade.[4,5] It is also clear that for the last few resonances, which are not as sharply defined (near $E \approx 2$), the total charge increases by less than one electron at a time, and also exhibits a gradual increase with energy in that range (no more strictly-flat plateaus).

The gradual change of the charge is characteristic of the case when the resonances are not sharp. A more extreme example of this is shown in Fig. 2(a), where for $\beta_0 = \beta_L = 1$ one finds strongly overlapping resonances even for the noninteracting case. The charge density in this case is only vaguely reminiscent of the steplike structure, and is well below the expected value of 6 after the first six resonances shown in that figure.

In Fig. 2(b), we show a case where the length of the in-

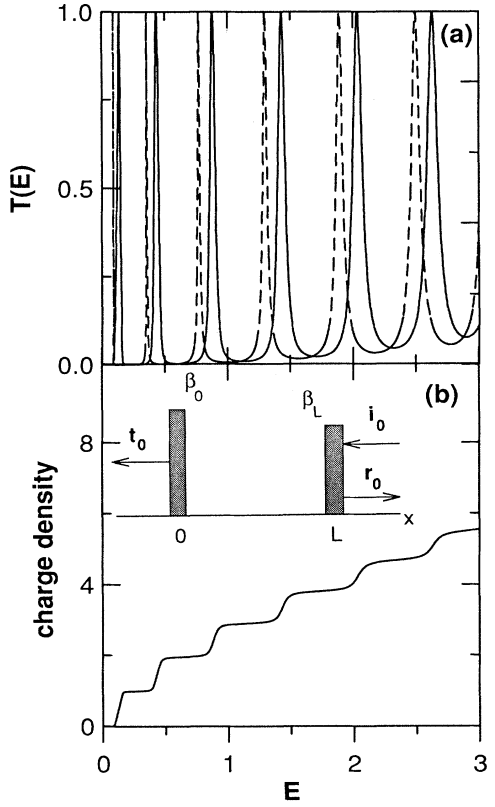

FIG. 1. (a) Transmission coefficient as a function of energy for the case $L = 10$, $\beta_0 = \beta_L = 5$, showing the effects of interaction with $U = 0.5$ (solid line). The noninteracting case $U = 0$ is also shown (dashed line). (b) Total charge density accumulated in the well as a function of energy. Inset: schematic representation of the model and notation.

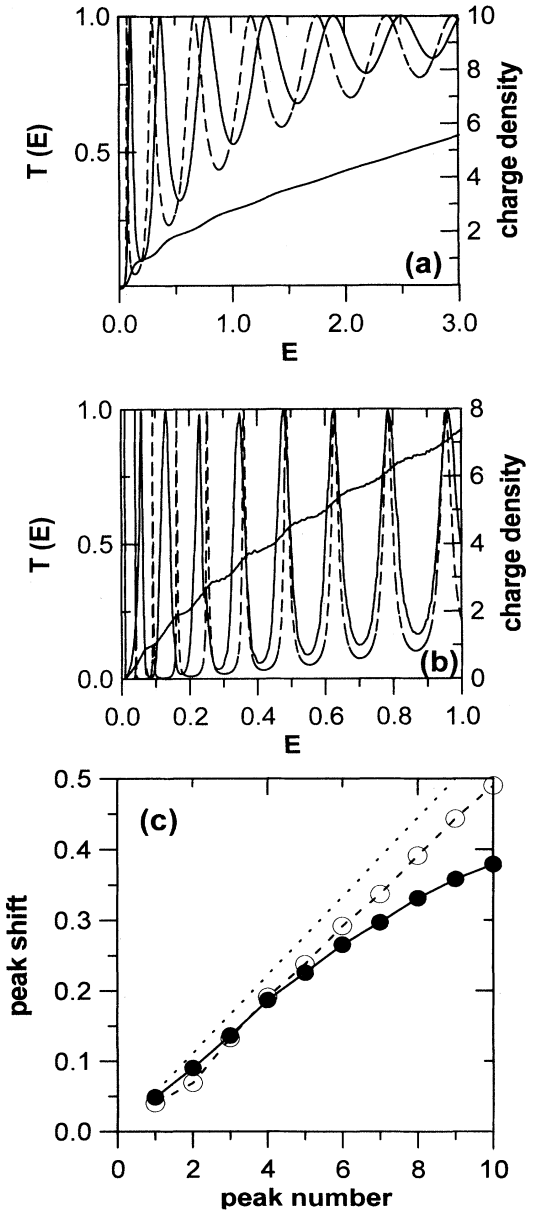

FIG. 2. (a) Interaction effects on the transmission coefficient for $L = 10$, $\beta_0 = \beta_L = 1$, and $U = 0.5$, and corresponding charge density, as a function of energy. (b) $L = 30$, $\beta_0 = \beta_L = 2$, and $U = 5/3$. Solid curves include interactions; dashed curves do not. (c) Resonance peak shifts versus the peak number for the case in (b). The dashed line (○) denotes the "ideal" shift, $U\bar{\rho}$; dotted line has slope U/L. The solid line (•) shows actual calculated shifts.

teraction region is larger, so that the resonances are quite sharp and close in energy ($L = 30$, $\beta_0 = \beta_L = 2$). For this case, we have also used a larger value of the effective interaction constant, $U = 5/3$, and the resonance shifts are proportionally larger, for the most part. Here, the computation time increases significantly, as the perturbation given by the interaction is larger and finer sweeps of the energy have to be used to obtain reliable and well-converged results. This figure shows eight shifted peaks for $E \leq 1$, in the same region where ten resonances exist for the noninteracting system. The larger shifts are of course produced by a larger value of U, although the details are related to the charge profiles: One would anticipate that as the first resonant quasibound state is below the incident energy, the charge would accumulate with an envelope function which approximately follows a squared-sine profile. [This follows if one considers that the lowest trapped state in a quantum well has only nodes at the ends of the well. The finite lifetime associated with the resonance width changes the wave function profile only slightly, especially for high barriers or sharp resonances. One can verify that this is indeed the case by inspection of the resulting c_i coefficients obtained in our solutions (not shown).] However, as more charge accumulates in the well, the charge is distributed more homogeneously and the peak shifts become proportional to the charge number.

One can analyze in more detail the different resonance shifts. One would expect that each shift is approximately equal to $U\overline{\rho}$, where $\overline{\rho} = L^{-1}\sum_i \rho_i$ is the value of the average charge density *at the energy of the shifted resonance.* This assumes that the charge is distributed homogeneously in the well, which would in turn result in the bottom of the well being shifted upwards equally at every site/position. As we see in Fig. 2(c), this is not what one obtains [the peak shifts shown are for the case in Fig. 2(b)]. The difference between the calculated shift (solid line and symbols) and the expected value given above ($U\overline{\rho}$) is first small for small total charge values, but it increases for larger energy or charge values. Notice, moreover, that the calculated shift is at first higher than the estimated average value. This is due to the piling up of the charge in the central portion of the well, as discussed above. The larger value of the Coulomb "charging" energy is then a direct consequence of the microscopic details of the electronic wave function. Possible evidence of this behavior is seen in the capacitance measurements of Ashoori *et al.*,[10] where the first few "charging peaks" are spaced a bit more than subsequent ones. (The identification of resonance peaks with the magnetocapacitance features in experiments should be valid for narrow resonances, as they would evolve into the "addition spectrum" of the true eigenstates of a closed system.)

We have also noticed in all the cases studied that the shift is always much smaller than multiples of U/L [shown as dotted line in Fig. 2(c)], as the classical model predicts for $U \gg \Delta\epsilon$. In fact, it is evident in Fig. 2(c) that there is an overall *decrease* of the calculated resonance shift for higher resonances (or higher energy). This is a more subtle consequence of the shape of the wave functions producing the shifts in the calculation. As the energy of incidence increases and the resonances begin to overlap more and more, the charge in the well no longer increases in a steplike fashion, as shown above. This is due, in the language of wave functions, to the fact that as the barriers are effectively more transparent at that energy, the fractional weight of the wave function trapped in the well is smaller. Correspondingly, the change in the local potential decreases relatively to the incident energy and so do the shifts. Notice that although we use a constant value of the *on-site* repulsion energy U, the self-consistent calculation of the resonant structure effectively reduces the importance of the interaction, via the decreasing wave function weights. This approach, therefore, describes an effectively decreasing interaction for states closer to the top of the barrier, as one would expect on physical grounds: For sufficiently transparent barriers (or high energies here), the transport through this region would become ideal (and yield the proper Ohmic limit when dissipation is included[30]).

In conclusion, we have studied the problem of charging in a double-barrier structure. The repulsive interaction arising from the charge accumulation shifts the resonance structures in the transmission coefficient depending on the microscopic details of the resonant wave function. The shifts decrease for increasing transparency of the barriers. Our approach is intuitive, computationally simple, and yields the expected limiting results. We are currently in the process of studying the effects of barrier asymmetry (found to be important in many experiments),[20,22] and finite bias.[27] We will report these results elsewhere.

This work was supported in part by CONACYT Project No. 3536–E9311, and the US DOE Grant No. DE–FG02–91ER45334. S.E.U. acknowledges support by the A. v. Humboldt Foundation. E.C. acknowledges gratefully the hospitality of the Department of Physics and Astronomy at Ohio University, and the technical support of A. Reyes at IFUNAM–Ensenada.

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