Correlation effects on transport through few-electrons systems

J. J. Palacios(∗), L. Martin-Moreno(∗∗) and C. Tejedor(∗)

(∗) Departamento de Física de la Materia Condensada.
Universidad Autónoma de Madrid.
Cantoblanco, 28049, Madrid. Spain.

(∗∗) Instituto de Ciencia de Materiales (CSIC)
Universidad Autónoma de Madrid.
Cantoblanco, 28049, Madrid. Spain.

March 23, 2022

Abstract

We study lateral tunneling through a quantum box including electron-electron interactions in the presence of a magnetic field which breaks single particle degeneracies. The conductance at zero temperature as a function of the Fermi energy in the leads consists of a set of peaks related to changing by one the electron occupancy in the box. We find that the position and heights of the peaks are controlled by many-body effects. We compute the conductance up to 8 electrons for several cases where correlation effects dominate. In the range of intermediate fields spin selection rules quench some peaks. At low and high fields the behavior of the conductance as a function of the number of electrons is very different due to big changes in the many-body ground state wavefunctions.
The increasing ability for producing extremely small cavities where only a few electrons ($N \leq 10$) coexist, allows the study of many-body effects on the lateral tunneling through such structures\cite{1}. The concept of capacitance is too simple to describe effects, like exchange and correlation, which should be extremely important in these small systems. In many cases, the experiments are performed in the presence of a high magnetic field $\mathbf{B}$. The aim of this paper is to show that correlation effects are crucial, even in the case in which the system is not in the fractional quantum Hall regime. A Keldysh framework \cite{2} is used to obtain the conductance of a square quantum box, in the linear response regime, including electron-electron interaction. The leads are assumed to behave like a Fermi liquid, \textit{i.e.}, electrons there can be described in terms of quasiparticles. Hartree, exchange and correlation interactions among all the electrons confined in the box are included in order to calculate conductances. We include a cut-off in the two-dimensional Coulomb interaction to take into account the finite width of actual systems.

We analyze lateral magnetotunneling including many body effects in the dot by using a Keldysh formalism \cite{2},\cite{3},\cite{4}. We take two equal barriers separating the box from each lead. So, the current is given by \cite{3}

$$J = \frac{-2e}{\hbar} \int d\omega \left[ f_L(\omega) - f_R(\omega) \right] \text{Im} \left[ \text{tr} \{ \Gamma G^r \} \right]$$

where $f_L$ and $f_R$ are the Fermi distributions of the left and right leads respectively and $G^r$ is the non-equilibrium retarded Green’s function including all the many body effects as well as the coupling to the leads given by $\Gamma$. In a single particle basis,

$$\mathcal{G}^r_{i,j}(t) = -i\theta(t) \left( \langle d_i(t) d_j^\dagger \rangle + \langle d_j^\dagger d_i(t) \rangle \right)$$

and

$$\Gamma_{i,j}(\omega) = 2\pi \sum_l \rho_l(\omega) \langle i | V | l \rangle \langle l | V | j \rangle.$$
$d_i$ and $d_j^\dagger$ are the annihilation and creation operators of box states $|i\rangle$ and $|j\rangle$ respectively, the angular brackets in $G_{i,j}^r$ mean thermal average, $V$ is the potential that couples the box to the leads, these having eigenstates $|l\rangle$ and density of states $\rho_l$. It is important to realize that the coupling $\Gamma$ can be obtained as output of a single-particle calculation of tunneling.

We concentrate in the linear regime at zero temperature so that thermal averages become expectation values in the ground state, $G_r$ being the equilibrium retarded Green’s function at zero temperature. The total Hamiltonian is represented in the basis of antisymmetrized configurations $\alpha^{(N)} \equiv \{n_i\}$ where $n_i$ are the occupations of single particle states $|i\rangle$ verifying $n_i = 0$ or $1$ and $\sum_i n_i = N$. The many-body eigenstates with energies $E_{\beta}^{(N)}$ of a box with $N$ electrons are written as $\Phi_{\beta}^{(N)} = \sum_\alpha c_{\alpha,\beta}\alpha^{(N)}$. In this basis, the equilibrium Green’s function $g^r$ for an isolated box takes, in the Lehmann representation, the form

$$g_{i,j}^{r(N)}(\omega) = \lim_{\eta \to 0} \sum_\beta \left[ \frac{\Delta_{i,j}^{(N)\beta+}}{\omega + E_{\beta}^{(N)} - E_{\beta}^{(N+1)} + i\eta} + \frac{\Delta_{i,j}^{(N)\beta-}}{\omega - E_{\beta}^{(N)} + E_{\beta}^{(N-1)} + i\eta} \right]$$

where the numerators are spectral weights $\Delta_{i,j}^{(N)\beta+} = \langle \Phi_0^{(N)} | d_i | \Phi_{\beta}^{(N+1)} \rangle \langle \Phi_{\beta}^{(N+1)} | d_j^\dagger | \Phi_0^{(N)} \rangle$ and $\Delta_{i,j}^{(N)\beta-} = \langle \Phi_0^{(N)} | d_i^\dagger | \Phi_{\beta}^{(N-1)} \rangle \langle \Phi_{\beta}^{(N-1)} | d_j | \Phi_0^{(N)} \rangle$. The calculation of the conductance $G = eJ/\Delta \mu$, requires the coupling to the leads by using a selfenergy $\Sigma^r = (g^r)^{-1} - (G^r)^{-1}$. The interaction and the coupling to the leads must be solved simultaneously. Such an analysis has been only done for the Anderson Hamiltonian[4],[5],[6]. A Kondo-like peak appears in the density of states at the Fermi energy and at zero temperature due to correlations to the leads. This would give rise to a perfect transparency. The existence of the Kondo effect requires degeneracy, usually of spin, of the single-particle levels. If the degeneracy is broken by the Zeeman term due to magnetic field, the Kondo peak shifts away from the Fermi energy and, again, correlations to the leads are not important for the properties at such energy[5]. Therefore, in our problem with magnetic field, we neglect correlations in the coupling to the leads and consider the selfenergy $\Sigma^r$ only as the non-interacting, single-particle selfenergy $\Sigma^{sp}$. A very good approximation for the single-particle selfenergy is to consider that the coupling to
the leads only broadens the levels \( i, j \) but does not shift or mix them, \( i.e. \Sigma_{i,j}^{sp} \approx -i\Gamma_{i,j}\delta_{i,j} \).

Then, the conductance in the presence of the magnetic field becomes

\[
G = \frac{e^2}{h} \sum_{N,i} \left[ \frac{\Delta^{(N)+}_{i,i} + \Gamma^2_{i,i}(E_F)}{\left( E_F - \delta V - E_0^{(N+1)} + E_0^{(N)} \right)^2 + \Gamma^2_{i,i}} + \frac{\Delta^{(N)-}_{i,i} - \Gamma^2_{i,i}(E_F)}{\left( E_F - \delta V + E_0^{(N-1)} - E_0^{(N)} \right)^2 + \Gamma^2_{i,i}} \right]
\]

where, for zero temperature and well resolved resonances, the only significant contribution comes from \( \beta \equiv 0 \). \( E_F \) is the Fermi level of the leads and \( \delta V \) gives the bottom of the box potential with respect to those of the leads. The conductance reduces to a set of peaks, each one related to the variation of the discrete number \( N \). This is achieved when the Fermi level at the leads verifies \( E_F \approx \delta V \pm E_0^{(N\pm1)} \pm E_0^{(N)} \). The position of each peak of the conductance is a many-body feature, a result also obtained in the very different regime \( k_B T \gg \Gamma \). Correlation effects reflect on the height of each peak, which is given by \( \sum_i \Delta^{(N)}_{i,i} \). The width of each peak is given by the single particle coupling \( \Gamma_{i,i} \).

We apply the above discussed scheme to a square box defined by two barriers built up in a wire (along the \( y \) direction) of width \( W \) by means of transversal (i.e. in the \( x \) direction) gate potentials. These gate potentials create two effective barriers of width \( l_b \) and height \( V_b \) separated from each other by the distance \( W \). In such a square geometry, only solutions for isolated boxes with \( N = 2 \) and \( B = 0 \) have been calculated. We work with a strong perpendicular magnetic field described in a Landau gauge (\( \vec{A} = Bx\hat{u}_y \)). Each single particle state will be labelled as \( \epsilon \equiv (n, k, \sigma) \) where \( \sigma \) is the spin index and \( n \) and \( k \) are the discrete quantum numbers related to spatial shape of the wavefunction. These single particle states are straightforwardly obtained from the diagonalization of the Hamiltonian represented in a basis of sines and cosines in the \( x \) and \( y \) directions. From these wavefunctions, the broadenings \( \Gamma_{i,i} \), required for the calculation of the conductance, are obtained using their expressions given before.

We present here results of the calculation for a square box of side \( W = 100 nm \). We use its single particle eigenfunctions to describe electron-electron interactions within the
box. The calculation of each matrix element of the total Hamiltonian reduces to compute four-dimensional integrals involving single particle wave functions. By diagonalizing the Hamiltonian one obtains the energies of \( N \) electrons in the box as well as the eigenstates in the form of linear combinations of configurations. The box is defined by two barriers of width \( l_b = 25 \text{nm} \). In order to have weak coupling between the box and the leads we take a barrier height \( V_b = 12 \text{meV} \). Following the experimental procedure, we fix the Fermi energy of the leads at \( E_F = 11.5 \text{meV} \) and move the box bottom potential \( \delta V \).

There are three regimes of \( B \) depending on the characteristics of the many-body ground states. First, we present results in the intermediate regime of magnetic fields. The main result is that the ground state of the box with \( N \) electrons change its multiplet symmetry when varying the magnetic field. This has an important implication: for some ranges of \( B \) the difference between the total spin of \( N \) and \( N \pm 1 \) electrons is larger than \( 1/2 \). Then, the spectral weights are zero and the conductance of the box when passing from \( N \) to \( N + 1 \) electrons disappears. Later on, following with the variation of the field, the multiplet character of the ground state changes once again and the difference \( 1/2 \) is restored and the peak of the conductance appears once again. This is observed in figure 1 in the conductance of our square box with magnetic fields corresponding to have 5, 6 and 7 flux quanta through the box (this implies to cover a range between 2 and 3\( T \)). Since we fix the energy difference between the top of the barrier and the Fermi energy of the leads, the broadening of all the peaks is practically the same. The numbers within the figure stand for the number of electrons within the box. For the lower field, the conductance decreases when \( N \) increases, due to the decrease of the spectral weights. When the magnetic field increases, the peak corresponding to 4 electrons disappears because the ground state of 3 electrons has a total spin \( S = 3/2 \) while the ground state of 4 electrons has a total spin \( S = 0 \) so that the spectral weight is zero. This gives a zero in the conductance intensity although a small lowering of the bottom of the dot potential would allow the introduction of the electron in the dot without implying...
current \((i.e.\ \text{conductance})\) in the whole system. For an even higher field, the ground state of the dot with 3 electrons recovers \(S = 1/2\) and the peak conductance corresponding to 4 electrons appears once again. Apart from selection rules as the above discussed, the peak heights are given by the spectral weights \(\Delta_{i,i}^{(N)}\) obtained from the \(N\)-electrons wave functions of the box. At the higher field, the peak corresponding to 2 electrons becomes rather small because the ground state corresponds to single particle wavefunctions in the outer region of the box due to Coulomb repulsion while the 1 electron ground state is situated in the inner region so that the spectral function reduces significantly. This is similar to the orbital angular momentum rule obtained in circular dots\([3],[9]\). The peaks have been shifted with respect to the single particle result by the charging effect that, in this case, results to be rather constant with the number of particles.

Let us now discuss the high and low field regimes in which there are not questions related to total spin selection rules. Figure 2 gives the conductance of the box containing up to 8 electrons for magnetic fields in two different regimes. For 3 flux quanta through the box \((B = 1.25T)\) the many-body wavefunctions are rather complicated including all the possible spin configurations, while for 12 flux quanta \((B = 5T)\) the \(N\)-electrons ground state is spin polarized. Due to the big differences in the wavefunctions, the peaks behave in a very different way. For the lower field \((i.e.\ \text{for non-polarized wavefunctions})\) the peak show a monotonous decrease with increasing \(N\). On the contrary, for the higher field \((i.e.\ \text{for spin polarized wavefunctions})\) the spectral weights are such that, after having a minimum, the peaks tend to have a conductance \(e^2/h\). It must be stressed that we are presenting conductances coming from ground state properties at fixed magnetic field, something different to previous works\([3]\) where, in order to study the fractional regime, the system is not maintained in its ground state. Some other minor results can also be drawn from figure 2: 1) the charging energy is not totally constant and 2) for the high field, once again, the peak for 2 electrons is very small because it relates \(N\)-electron wavefunctions with very different spatial distribution.
In summary, we have computed the conductance of a box in the presence of a magnetic field at zero temperature including all the electron-electron interaction without any restriction in the spin configuration. The conductance consists of a set of peaks with their position and intensity determined by many-body effects while their width is essentially given by the coupling between single particle states in the box and in the leads. In the intermediate range of fields, the ground state of \( N \) electrons change its multiplet character with the variation of the magnetic field implying selection rules that quench some conductance peaks. The ground state wavefunctions have big differences between the low and the high field regimes. Therefore, the spectral weights imply very different behavior of the conductance peaks as a function of the number of electrons in both field regimes.

This work has been supported in part by the Comision Interministerial de Ciencia y Tecnologia of Spain under contracts MAT 91 0201 and MAT 91 0905-C02-01 and by the Commission of the European Communities under contract SSC-CT90-0020.

References

[1] M. A. Kastner, Phys. Today, January 1993, p. 24 and references therein.

[2] Y. Meir and N. S. Wingreen, Phys. Rev. Lett. 68, 2512 (1992).

[3] J. M. Kinaret et al., Phys. Rev. B 45, 9489 (1992); ibid. 46, 4681 (1992).

[4] S. Hershfield, J. H. Davies and J. W. Wilkins, Phys. Rev. B 46, 7046 (1992).

[5] T. K. Ng and P. A. Lee, Phys. Rev. Lett. 61, 1768 (1988); L. I. Glazman and M. E. Raikh, JETP Lett., 47, 452 (1988).

[6] Y. Meir, N. S. Wingreen and P. A. Lee, Phys. Rev. Lett. 66, 3048 (1991).

[7] C. W. J. Beenakker, Phys. Rev. B 44, 1646 (1991); C. W. J. Beenakker, H. van Houten and A. A. M. Staring, Phys. Rev. B 3819 (1992).
[8] G. W. Bryant, Phys. Rev. Lett. 59, 1140 (1987); W. Hausler, B. Kramer and J. Masek, Z. Phys. B 85, 435 (1991); T. Brandes, W. Hausler, K. Jauregui, B. Kramer and D. Weinmann, preprint.

[9] P. A. Maksym and T. Chakraborty, Phys. Rev. Lett. 65, 108 (1990); Phys. Rev. B 45, 1947 (1992); U. Merkt, J. Huser and M. Wagner, Phys. Rev. B 43, 7320 (1991).
FIGURE CAPTIONS

Figure 1. Many-body conductance $G$ of a box with $W = 100\,nm$ and $E_F = 11.5\,meV$ as a function of the dot bottom potential between $B = 2$ and $3T$.

Figure 2. Many-body conductance $G$ of a box with $W = 100\,nm$ and $E_F = 11.5\,meV$ as a function of the dot bottom potential for $B = 1.25$ and $5T$. 