Medium/high field magnetoconductance in chaotic quantum dots

E. Louis
Departamento de Física Aplicada, Universidad de Alicante, Apartado 99, E-03080 Alicante, Spain.

J. A. Vergés
Instituto de Ciencia de Materiales de Madrid, Consejo Superior de Investigaciones Científicas, Cantoblanco, E-28049 Madrid, Spain.

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The magnetoconductance $G$ in chaotic quantum dots at medium/high magnetic fluxes $\Phi$ is calculated by means of a tight binding Hamiltonian on a square lattice. Chaotic dots are simulated by introducing diagonal disorder on surface sites of $L \times L$ clusters. It is shown that when the ratio $W/L$ is sufficiently large, $W$ being the leads width, $G$ increases steadily showing a maximum at a flux $\Phi_{\text{max}} \propto W$. Bulk disordered ballistic cavities (with an amount of impurities proportional to $L$) does not show this effect. On the other hand, for magnetic fluxes larger than that for which the cyclotron radius is of the order of $L/2$, the average magnetoconductance increases almost linearly with the flux with a slope proportional to $W^2$, shows a maximum and then decreases stepwise. These results closely follow a theory proposed byBeenakker and van Houten to explain the magnetoconductance of two point contacts in series.

I. INTRODUCTION

Magnetococonductance in chaotic quantum dots have attracted a great deal of attention in recent years [1–4]. Weak localization effects have been thoroughly investigated searching for differences between chaotic and regular cavities [11,12]. More recently the selfsimilar character of magnetoconductance fluctuations in chaotic quantum dots has deserved several experimental studies [13,14]. In Ref. [4] it was reported that in cavities with sufficiently soft walls, rather wide leads and a high zero field conductance of the order of 40 conductance quanta, fluctuations were very weak and the magnetoconductance increased steadily in approximately 20% over 50 flux quanta [14]. Although an increase in the magnetoconductance as a function of the magnetic flux in cavities with wide leads may not be that surprising, no theoretical analysis of this result is yet available. This is so despite of the wealth of experimental and theoretical information on magnetoconductance in related mesoscopic systems [15,16].

The purpose of the present work is to investigate the magnetoconductance of chaotic quantum dots over a wide range of magnetic field. Quantum dots are described by means of a tight-binding Hamiltonian on $L \times L$ clusters of the square lattice. Non–regular (chaotic) behavior is induced by introducing disorder at surface sites, a procedure that has been shown to reproduce all properties of quantum chaotic cavities [12]. The most outstanding conclusions derived from our study are the following. For sufficiently open systems, large leads width $W$ or, alternatively, high zero field conductance, the magnetoconductance increases steadily as a function of the magnetic flux, reaching a maximum at a magnetic flux $\Phi_{\text{max}}$ proportional to the leads width. This effect, which is in agreement with the experimental observations of [14], does not show up in regular or bulk disordered cavities. The average magnetoconductance versus magnetic flux curve shows four clearly differentiated regions: i) At small fluxes (typically below 1–2 flux quanta) the weak localization peak with the typical Lorentzian shape is observed. ii) This is followed by a flux range over which the magnetoconductance shows a non–universal behavior which depends on leads configuration. iii) The latter lasts until the cyclotron radius becomes of the order of $L/2$. Beyond this point the average magnetoconductance increases linearly with the magnetic flux with a slope which increases with the leads width (for very small $W$ the slope is nearly zero and the magnetoconductance remains constant in a large flux range) . iv) At large fluxes the magnetoconductance decreases stepwise (each step of one flux quantum), due to the successive crossings of the Fermi energy of the transversal modes that contribute to the current. As discussed below these results are compatible with a theory proposed by Beenakker and van Houten [17] to interpret the experimental results for the magnetoconductance of two point contacts in series [14].

The rest of the paper is organized as follows. Section II includes a description of our model of chaotic quantum dot and of the method we used to compute the current. The results are presented in Section III, and discussed in terms of the theory of Ref. [11] in Section III. Section IV is devoted to summarize the conclusions of our work.

II. MODEL AND METHODS

A. Model

The quantum dot is described by means of a tight-binding Hamiltonian with a single atomic level per lattice
site on $L \times L$ clusters of the square lattice:

$$
\hat{H} = \sum_{m,n < IS} \omega_{m,n} |m,n \rangle \langle m,n| - \sum_{<m,n',n>} t_{m,n,m',n'} |m,n \rangle \langle m',n'|,
$$

(1)

where $|m,n \rangle$ represents an atomic orbital on site $(m,n)$. Indexes run from 1 to $L$, and the symbol $<>$ denotes that the sum is restricted to nearest-neighbors. Using Landau’s gauge the hopping integral is given by,

$$
t_{m,n,m',n'} = \exp \left( \frac{2\pi i m}{(L-1)^2} \right), \quad m = m', \quad \text{otherwise}
$$

(2)

where the magnetic flux $\Phi$ is measured in units of the quantum of magnetic flux $\Phi_0 = h/e$. The energy $\omega_{m,n}$ of atomic levels at impurity sites $(IS)$ is randomly chosen between $-\Delta/2$ and $\Delta/2$, whereas at other sites $\omega_{m,n} = 0$. Impurities were taken on all surface sites [11,13] but those coinciding with the leads entrance sites to avoid excessive (unphysical) scattering. This model has been proposed to simulate cavities with rough boundaries and its properties closely follow those characterizing quantum chaotic systems [11,13]. Some calculations were also carried out on clusters with 2$L$ bulk impurities [17].

B. Conductance

The conductance (measured in units of the quantum of conductance $G_0 = e^2/h$) was computed by using an efficient implementation of Kubo formula. The method is described in [14], while applications to mesoscopic systems can be found in [13,14]. For a current propagating in the $x$-direction, the static electrical conductivity is given by:

$$
G = -2 \left( \frac{e^2}{h} \right) \text{Tr} \left[ (\hbar \hat{v}_x) \text{Im} \hat{G}(E) (\hbar \hat{v}_x) \text{Im} \hat{G}(E) \right],
$$

(3)

where $\text{Im} \hat{G}(E)$ is obtained from the advanced and retarded Green functions:

$$
\text{Im} \hat{G}(E) = \frac{1}{2i} \left[ \hat{G}^R(E) - \hat{G}^A(E) \right],
$$

(4)

and the velocity (current) operator $\hat{v}_x$ is related to the position operator $\hat{x}$ through the equation of motion $\hbar \dot{\hat{x}} = \left[ \hat{H}, \hat{x} \right]$, $\hat{H}$ being the Hamiltonian. Numerical calculations were carried out connecting quantum dots to semiinfinite leads of width $W$ in the range $1 - L$. The hopping integral inside the leads and between leads and dot at the contact sites is taken equal to that in the quantum dot (ballistic case). Assuming the validity of both the one-electron approximation and linear response, the exact form of the electric field does not change the value of $G$. An abrupt potential drop at one of the two junctions provides the simplest numerical implementation of the Kubo formula [14] since, in this case, the velocity operator has finite matrix elements on only two adjacent layers and Green functions are just needed for this restricted subset of sites. Assuming this potential drop to occur at the left contact ($lc$) side, the velocity operator can be explicitly written as,

$$
\hbar \dot{v}_x = -\sum_{j=1}^{W} (|lc,j \rangle < 1,j| - |1,j \rangle < lc,j|)
$$

(5)

where $(|lc,j \rangle$ are the atomic orbitals at the left contact sites nearest neighbors to the dot.

Green functions are given by:

$$
|E\hat{I} - \hat{H} - \hat{\Sigma}_1(E) - \hat{\Sigma}_2(E)|\hat{G}(E) = \hat{I},
$$

(6)

where $\hat{\Sigma}_1,2(E)$ are the selfenergies introduced by the two semiinfinite leads [3]. The explicit form of the retarded selfenergy due to the mode of wavevector $k_y$ is:

$$
\Sigma(E) = \frac{1}{2} \left( E - \epsilon(k_y) - i \sqrt{4 - (E - \epsilon(k_y))^2} \right),
$$

(7)

for energies within its band $|E - \epsilon(k_y)| < 2$, where $\epsilon(k_y) = 2\cos(k_y)$ is the eigenenergy of the mode $k_y$ which is quantized as $k_y = (nk_y \pi)/(W+1), nk_y$ being an integer from 1 to $W$. The transformation from the normal modes to the local tight-binding basis is obtained from the amplitudes of the normal modes, $<n|k_y>$ = $\sqrt{2/(W+1)}\sin(nk_y)$. Note that in writing Eq. (6) we assumed that the magnetic field was zero outside the dot [3]. This point will have some relevance in relation to the interpretation of our numerical results in terms of the theory of Ref. [14].

Calculations were carried out on clusters of linear size $L = 47 - 394$ (in units of the lattice constant) and at a fixed arbitrarily chosen, Fermi energy $E = -\pi/3$. In some cases averages over disorder realizations were also done. Although most calculations were performed with input/output leads of width $W$ connected from site $(1,1)$ to site $(1,1+W)$, and from $(L,L)$ to $(L,L-W)$, respectively, other input/output leads configurations were also explored. All calculations on disordered systems were done at a fixed value of the disorder parameter $\Delta=6$.

III. RESULTS

We first discuss results for $W/L$ similar to that used in the experiments of Ref. [3]. In that work conductance measurements were taken on a stadium cavity with a lithographic radius of 1.1 $\mu$m and leads 0.7 $\mu$m wide, which gives a $W/L$ ratio of 0.64. Fig. 1 shows the results for the magnetocconductance in cavities of linear sizes in
the range $L=47–394$ and leads of width $W = 0.65L$. The results correspond to a single realization of disorder. The most interesting result is the steady increase of the conductance with the magnetic field. The conductance reaches a maximum at a magnetic flux which, as illustrated in the inset of the Figure, increases linearly with the leads width, or the linear size of the system. Note that, as the results of Fig. correspond to $W \propto L$, they cannot allow to identify which of the two parameters ($W$ and $L$) control the maximum in $G$. We have checked, however, that it is in fact $W$ the one that matters (see also below). The increase in $G$ until the maximum is reached can be as high as 30%. It is interesting to remark that the increase in the conductance occurs with relatively small fluctuations due to the large $W/L$ ratio (or degree of opening) of the cavity (see (16)). Although the experimental data were taken at fields not high enough to observe the maximum shown in Fig. it can be safely assessed that our results are compatible with those of Ref. (14). In particular the zero field conductance reported in that work was around 38 quanta, increasing up to 46 quanta over approximately 50 flux quanta. This is rather similar to the magnetoconductance curve for $L = 197$ shown in Fig. (1).

In Fig. we compare the results for the cavity with surface disorder with those for a regular cavity and for a cavity with $2L$ bulk impurities. The results indicate that the cavity having surface disorder is the only one that reproduces the experimental results (14). In regular cavities the conductance does not increase steadily due to the large amplitude oscillation discussed in (16). This behavior clearly differentiates regular and chaotic cavities. At large fields the result for the cavity with surface disorder coincides with that for the regular cavity. This is a consequence of the fact that for sufficiently high fields the current is dominated by edge-like states which are not affected by surface disorder. semiclassically one can view carriers motion as short orbits bouncing off the same boundary. The associated quantum states have chirality and are thus commonly refer to as chiral states or edge states. The stepwise decrease of the magnetoconductance observed in regular and chaotic cavities with surface disorder is a consequence of the overall depopulation of Landau levels. It is interesting to note that the cavity with bulk disorder shows a markedly different behavior as this type of disorder can, instead, scatter carriers between opposite sides of the cavity. The results shown in Fig. illustrate the only difference we have found up to now between cavities with surface impurities or with a number of bulk impurities proportional to $L$ (18). Appart from this difference the two behave much alike and in line with what one expects to be the behavior of quantum chaotic cavities (3).

We have investigated how this steady increase of the magnetoconductance is affected by the leads width. In order to reduce fluctuations, which are particularly im-

\[ r_c = \frac{h\nu(E)}{4\pi} \frac{(L-1)^2}{\Phi_0} \Phi, \]  

where $h\nu(E) = \langle 2\sqrt{\sin^2 k_x + \sin^2 k_y} \rangle_E$. At the energy chosen here $h\nu(E) \approx 2.2$ (13). Then the flux at which $r_c = L/2$ is, for the size of Fig. $\Phi = 17\Phi_0$, which is very close to the flux at which the mentioned crossover occurs.

Fig. shows the averaged magnetoconductance for cavities of linear size $L = 47$ and leads widths in the range $W=4–20$. It is noted that the linear behavior discussed above appears in all cases at roughly the same magnetic flux indicating that it is only related to the cavity size $L$, as suggested by the discussion above. Instead the slope increases with the leads width. At small $W$ (systems with a low conductance) the conductance increases very slowly as a function of the magnetic flux. For sufficiently large $W$ the conductance reaches a maximum and then decreases stepwise. As remarked above, the latter is a consequence of the overall depopulation of transversal modes (or Landau levels). The slope of the linear part of the magnetoconductance is plotted as a function of leads width in Fig. The results can be accurately fitted by a $W^2$ law. The increase of the magnetoconductance can be understood in terms of the increase of the transmission probability of the transversal modes as their edge-like character increases and, consequently, its sensitivity to surface disorder is reduced. The steady increase in the conductance takes place until the mentioned depopulation begins to reduce the number of modes that participate in the current. Although this argument seems plausible, it cannot explain quantitative features of the results such as the linear relation between the conductance and the flux or the increase of the slope as the square of the leads width. This issue is addressed in the following Section.
IV. DISCUSSION

The results discussed in the previous subsection resemble those predicted by Beenakker and van Houten for the magnetoconductance of two point contact in series [10] and the related experiments of Staring et al [9]. Under the hypothesis that transmission between point contacts occurs with intervening equilibration of the current–carrying edge states, the authors of [9] derived the following expression for the conductance (in the following we take the conductance and flux quanta $G_0 = \Phi_0 = 1$ and do not include spin degeneracy),

$$G(\Phi) = \left[ \frac{1}{N_1} + \frac{1}{N_2} - \frac{1}{N_L} \right]^{-1}$$

where $N_i$ are the number of occupied subbands in the two contacts or leads ($i = 1, 2$) and in the region between the contacts, or in the present case in the dot ($i = L$). Disregarding discretness [10], $N_i$ can be written as,

$$N_i = \frac{n_i}{2\pi f(\xi_i)}$$

where the function $f(\xi_i)$ is,

$$f(\xi_i) = \begin{cases} \frac{2}{\pi} \arcsin \xi_i + \xi_i (1 - \xi_i^2)^{1/2}, & \text{if } \xi_i < 1 \\ 1, & \text{if } \xi_i > 1 \end{cases}$$

with $\xi_i = l_i/2r_c$, $l_i$ being a characteristic linear dimension in the three regions, in the present case, $l_i = W_1, W_2, L$.

We have used Eqs. (9) and (10) to fit the numerical results of Fig. 4. We took as fitting parameter the density or the Fermi velocity, $\hbar v = 2\sqrt{2\pi n}$, and assumed the same density in the leads and dot. As shown in Fig. 7 a satisfactory fitting is obtained for $\hbar v = 3.65$, almost twice the actual Fermi velocity in our model (see above). The theory reproduces the three regions that characterize our numerical results: an almost constant $G$ for small flux or $r_c > L/2$, a steadily increasing $G$ up to $r_c \approx W/2$ followed by a steep decrease at higher fluxes. It is interesting to note that the theory of Ref. [10] show a better agreement with the numerical results for the case in which the leads are attached at opposite corners of the dot, than with those for the other two lead configurations of Fig. 3. A possible reason for this behavior relies upon the equilibration assumption in Beenakker and van Houten theory. Equilibration is most likely when the leads are not facing each other, as is the case of leads attached to opposite corners. Instead, when leads are attached at contiguous corners direct transmission is more probable and equilibration requires higher magnetic fields to take place. This is a pictorial illustration of the assumptions under which the theory of Ref. [10] holds.

In order to check whether a linear relationship between the conductance and the flux in a rather wide range of fluxes, as indicated by the fittings of Fig. 4, can be understood in terms of this theory, we have expanded the conductance for small $\xi$ and $\xi_L > 1$. The result for leads having the same width and the same Fermi velocity (or density) in the leads and dot, is

$$G(\Phi) \approx \frac{n_1}{2\pi B} \left[ 2\xi + \frac{4}{\pi} \xi^2 + \left( \frac{8}{\pi^2} - \frac{1}{3} \right) \xi^3 \right]$$

As the maximum in $G$ occurs for $\xi$ slightly smaller than unity, checking whether $G$ varies linearly with the magnetic field below the maximum requires only to calculate the ratio between the coefficients of the second and third power of $\xi$ in Eq. (12). This ratio is 2.82, indicating that the linear term dominates in agreement with our numerical results. This equation also shows that the slope of the straight line is proportional to $W^2$. To make a quantitative comparison with the result of Fig. 5 we rewrite Eq. (12) introducing the actual expression for the ratio between the coefficients of the second and third power of $\xi$; the result is,

$$G(\Phi) \approx \frac{\hbar v}{4\pi} W + \frac{W^2}{2\pi L^2} + \frac{\pi}{2\hbar v} \left( \frac{8}{\pi^2} - \frac{1}{3} \right) \frac{W^3}{L^2}$$

The coefficient of the linear term results to be $1.44 \times 10^{-4} W^2$ not too far from the numerical result of Fig. 5.

Before ending it is worth to comment on several differences between our model calculation and the theory of Ref. [10]. We first note that we have assumed that the magnetic field is zero outside the dot, which may at first sight invalidate the use of Eq. (10). Nevertheless, the Green function of the whole system is calculated through Dyson’s equation (see Eq. 6). This means that the region of the leads close to the dot is distorted by the magnetic field, which seems to be enough to validate the calculation of the number of occupied subbands by means of Eq. (10). On the other hand whereas in the theory of Ref. [10] each channel contributes with one quanta to the conductance, in our case this contribution is approximately halved (remember that we work on chaotic cavities, see Ref. [6]). This seems, however, to be irrelevant as far as the qualitative behavior of the conductance is concerned.

V. CONCLUDING REMARKS

Summarizing, we have presented a numerical analysis of the magnetoconductance of quantum chaotic cavities in a wide range of magnetic fields. For sufficiently open cavities the magnetoconductance increases steadily reaching a maximum at a flux proportional to the leads width. This steady increase of $G$ agrees with the experimental observations reported in [6]. Neither regular nor bulk disordered cavities behave in this way. Numerical results for the average magnetoconductance indicate that, for magnetic fluxes larger than that for which the
The cyclotron radius is approximately $L/2$ and smaller than the flux at which the mentioned maximum is reached, it increases linearly with the magnetic flux $\Phi$ with a slope proportional to the square of the leads width. At higher fluxes the conductance decreases stepwise. These results admit a satisfactory explanation in terms of the theory proposed by Beenakker and van Houten to interpret the experimental results for the magnetoconductance of two contacts in series. The fact that our results for small magnetic fluxes ($r_c > L/2$) show a better agreement with the theory in the case that the two contacts are attached to opposite corners of the dot (and, thus, are not facing each other), is related to the stronger equilibration of edge–states promoted by this lead configuration with respect to the other two geometries explored in this work.

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FIG. 2. Magnetoconductance versus magnetic flux (both in units of their respective quanta) in $97 \times 97$ dots with leads of width $W = 57$ connected at opposite corners of the dot. The results correspond to dots with: i) no disorder (broken line), ii) Anderson impurities with $\Delta = 6$ (a single realization of disorder) placed either on all surface sites but those coinciding with the leads entrance sites (continuous line) or $2L$ impurities distributed randomly within the dot (thin continuous line).

FIG. 3. Magnetoconductance versus magnetic flux in cavities of linear size $L = 47$ and leads of width $W = 4$ (triangles), 8 (diamonds), 12 (crosses), 16 (circles) and 20 (+), connected at opposite corners of the dot. Anderson impurities with $\Delta = 6$ were placed at all surface sites but those coinciding with the leads entrance sites. The results correspond to an energy $E = -\pi/3$ and an average over 600 disorder realizations. Straight lines were fitted for fluxes above 20 and below the flux at which the conductance shows a maximum. The slopes of the straight lines are plotted as a function of $W^2$ in Fig. 5.

FIG. 4. Magnetoconductance versus magnetic flux in cavities of linear size $L = 47$ and leads of width $W = 4$ (triangles), 8 (diamonds), 12 (crosses), 16 (circles) and 20 (+), connected at opposite corners of the dot. Anderson impurities with $\Delta = 6$ were placed at all surface sites but those coinciding with the leads entrance sites. The results correspond to an energy $E = -\pi/3$ and an average over 600 disorder realizations. Straight lines were fitted for fluxes above 20 and below the flux at which the conductance shows a maximum. The slopes of the straight lines are plotted as a function of $W^2$ in Fig. 5.

FIG. 5. Slopes of the lines fitted in Fig. 4 versus the square of the leads width $W$. The fitted straight line is $-0.0019 + 2 \times 10^{-4}W^2$. 

$G(\Phi)$
FIG. 6. Fitting of the numerical results of Fig. 4 by means of the theory of Ref. [10], broken and continuous curves respectively (see text).