Transport through quantum rings

B A Z António¹, A A Lopes² and R G Dias¹

¹ Department of Physics, I3N, University of Aveiro, Campus de Santiago, Portugal
² Institute for Physics, University of Freiburg, Rheinstrasse 10, D-79104 Freiburg, Germany

E-mail: rdias@ua.pt

Received 9 March 2013, in final form 10 March 2013
Published 18 April 2013
Online at stacks.iop.org/EJP/34/831

Abstract
The transport of fermions through nanocircuits plays a major role in mesoscopic physics. Exploring the analogy with classical wave scattering, basic notions of nanoscale transport can be explained in a simple way, even at the level of undergraduate solid state physics courses, and more so if these explanations are supported by numerical simulations of these nanocircuits. This paper presents a simple tight-binding method for the study of the conductance of quantum nanorings connected to one-dimensional leads. We show how to address the effects of applied magnetic and electric fields and illustrate concepts such as Aharonov–Bohm conductance oscillations, resonant tunneling and destructive interference.

(Some figures may appear in colour only in the online journal)

1. Introduction

Constructing circuits using nanoscale components such as single electron transistors, single molecule devices, nanowires etc, seems to be the most plausible way of extending Moore’s law over the next few years. Electron transport in these circuits must be addressed in the quantum mechanical framework and surprising features (strongly contrasting with those of bulk electronic transport) are known to occur, e.g. Coulomb blockade [1], conductance quantization [2] and resonant tunneling [3]. Much of the underlying physics behind these phenomena can be explained in a simple way, at least qualitatively, by analogy with classical wave scattering and it is reasonable to expect growing attention to these basic notions of nanoscale transport in the curricula of undergraduate solid state physics courses.

One of the simplest and most interesting nanocircuits is the open ring, for its simplicity and non-local quantum effects. Particle waves incident in the ring travel by both arms of the ring and interfere constructively or destructively on their way out, depending on the magnetic flux encircled by the quantum ring and on the position of the contacts. This leads to the so-called Aharonov–Bohm conductance oscillations in the conductance [4, 5]. In this paper we present a simple method for the numerical calculation of the conductance through tight-binding clusters and apply it to the particular case of quantum rings taking into account the dependence on...
applied magnetic and electric fields. In particular, we discuss the Aharonov–Bohm conductance oscillations. The leads are assumed to be one-dimensional for simplicity. We avoid defining quantities such as Green’s functions or self-energies and the problem of determining the conductance is reduced to that of finding the solution of a system of $N + 2$ linear equations (where $N$ is the number of sites of the ring), so that this computational study can be carried out by an undergraduate student, after taking an introductory course in quantum mechanics.

The remaining part of this paper is organized in the following way. In section 2, we describe the Hamiltonian for the system of the cluster and leads. In section 3, we show how to reduce the determination of the conductance to finding the solution of a linear system of $N + 2$ equations. In section 4, we present the results for the conductance through tight-binding rings in the presence of magnetic flux and electric fields. Finally, in section 5 we draw our conclusions.

2. System

Our system is composed of a tight-binding cluster with $N$ sites connected to two semi-infinite 1D leads modeled as 1D tight-binding semi-chains (see figure 1) [6]. The system Hamiltonian is the sum of the leads and cluster Hamiltonians, $H_0$, and the coupling between each lead and the cluster, $V_{LR}$.

\[
H = H_0 + V_{LR},
\]

with

\[
H_0 = -\sum_{j=-\infty}^{0} (|j-1\rangle\langle j| + \text{H.c.}) - \sum_{j=N+1}^{\infty} (|j\rangle\langle j+1| + \text{H.c.}) + H_s,
\]

where $H_s$ is the single-particle Hamiltonian in the scattering region (the cluster) and $|j\rangle$ is the Wannier state localized on the atomic site $j$ (see [6] for an introduction to tight-binding models using the Wannier function basis). The leads connected to the cluster are considered ideal with nearest-neighbor hopping $t = 1$. The coupling $V_{LR}$ between the leads and the cluster is given by

\[
V_{LR} = -t_L |0\rangle\langle L| - t_R |R\rangle\langle N + 1| + \text{H.c.},
\]
where the hopping matrix elements \( t_L \) and \( t_R \) connect the left and right leads, respectively, to the cluster sites \( L \) and \( R \). The Hamiltonian of the cluster is

\[
H_S = \sum_j \epsilon_j |j\rangle \langle j| - \sum_{i,j \neq j} (t_{ij} e^{i\phi_{ij}} |i\rangle \langle j| + \text{H.c.}),
\]

where the indices \( i \) and \( j \) run over all cluster sites. For a general gauge and an arbitrary geometry of the cluster, the phase shifts \( \phi_{ij} \) in the hopping factors between sites \( r_i = a \) and \( r_j = b \) are determined from

\[
\phi_{ij} = -\frac{\epsilon}{\hbar} \int_a^b A \cdot dr,
\]

where the integral is a standard line integral of the vector potential \( A \) along the line segment that links sites \( a \) and \( b \).

In this paper, we exemplify the application of the numerical method using the particular case of the conductance through a tight-binding ring threaded by a magnetic flux. This is a well-studied case and the reader should see, for example, [7–9] for in-depth analyses of the tight-binding ring conductance. The tight-binding Hamiltonian of a ring of \( N \) sites enclosing an external magnetic flux can be expressed as

\[
H_S = \sum_{j=1}^N \epsilon_j |j\rangle \langle j| - \sum_{j=1}^N t (e^{i\phi_j/N} |j\rangle \langle j+1| + e^{-i\phi_j/N} |j+1\rangle \langle j|),
\]

where \( \phi' = \frac{2\pi \Phi}{\Phi_0} \) is the reduced flux, \( \epsilon_j \) is the on-site energy, \( t \) is the hopping integral between two nearest neighbor sites, and \( \Phi_0 = \hbar/e \) is the flux quantum [6]. A particular gauge was chosen such that the Peierls phases are all the same and, assuming that the on-site energies \( \epsilon_j \) are site independent, the tight-binding Hamiltonian becomes translationally invariant and therefore its eigenfunctions are given by

\[
|k\rangle = \frac{1}{\sqrt{N}} \sum_{j=1}^N e^{ikj} |j\rangle,
\]

where \( \{ |k\rangle \} \) is the momentum basis, \( N \) is the number of atoms in the ring, \( k \) is the particle momentum and \( \{ |j\rangle \} \) is the position basis of the atoms. The periodic boundary condition leads to the momentum’s quantization, \( k = \frac{2\pi m}{N}, \ m = 0, 1, 2, N - 1, \) and the eigenvalues of the Hamiltonian are given by

\[
E(k) = -2t \cos \left( k - \frac{\phi'}{N} \right),
\]

where we consider the on-site energies to be equal to zero. The flux shifts the energy dispersion curve, as shown in figure 2.

3. Quantum scattering, transmittance and conductance

In this section, we explain how to obtain the conductance expression for a tight-binding cluster connected to two semi-infinite (modeled as tight-binding chains) leads. Our approach requires only the understanding of the tight-binding model, which is usually introduced in an undergraduate solid state course (see [6, 10] for a discussion of tight-binding models). We therefore avoid use of Green’s functions that are present in more advanced conductance calculations such as the Meir–Wingreen formulation [11] (which is based on the non-equilibrium Green’s functions method and takes into account electronic interactions in the cluster) or the traditional quantum scattering approach [12, 13] (which is a one-particle description of scattering events due to potential barriers). Our approach is further simplified by the fact that the particles are confined to 1D leads, and consequently no angle dependence is present in the conductance expressions.
In nanoscale devices the wavelike nature of the electron must be taken into account. In this case the quantum scattering description of the transmission of a 1D particle across a structural or potential barrier is closely analogous to the Fresnel description of a plane light wave incident in a interface between two dielectric media. The wavefunction of a particle with momentum $k$ and energy $\epsilon_k$ is written as an incident wave plus reflected and transmitted waves with amplitudes $r(\epsilon_k)$ and $t(\epsilon_k)$, respectively, relative to the incident wave. The transmission probability for this incident wave is $|t(\epsilon_k)|^2$. The linear conductance $G(T)$ of non-interacting fermions is determined using the Landauer formula [14], which relates the transmission probability $|t(\epsilon)|^2$ with the linear conductance $G(T)$ of the non-interacting fermions at temperature $T$. This formula is explained in the following way. A single state with a momentum $k$ (and an energy $\epsilon_k = -2 \cos k$ of the band of a 1D lead) carries a current $e v_k / L$ where $v_k$ is the 1D velocity of the electron, $\hbar v_k = d\epsilon_k / dk$ and $L$ is the length of the lead. The contribution to the current of the positive velocity states in an interval $\Delta k$ is therefore $I_{\Delta k} = e / (\hbar L) \sum_{\Delta \epsilon} d\epsilon / dk$. Assuming $L$ very large, so that the $k$ values are effectively continuous, the summation over $k$ can be replaced by an integral $\int d\epsilon$ and converted into an integral over energy $\int d\epsilon = \int (d\epsilon / d\epsilon_k) d\epsilon_k$. In the final expression for the current, the two derivatives cancel each other and one has $I_{\Delta \epsilon} = (e/\hbar) \Delta \epsilon$ where $\Delta \epsilon$ is the energy interval corresponding to $\Delta k$. This result states that independently of the form of the 1D band, all energy intervals with the same width within the bandwidth contribute equally to the current. In the case of the 1D tight-binding chain, one has that the velocity of the electrons goes to zero as the energy approaches the top or the bottom of the band and therefore the contribution of an individual state to the current goes also to zero. This is, however, compensated by the fact that the density of states is inversely proportional to the velocity and therefore diverges as the energy approaches the top or the bottom of the band, compensating the smaller individual contribution of each state. The same reasoning is followed for negative velocity states which generate a current in the opposite direction. A finite bias implies that the chemical potential for electrons with positive or negative velocities is different (they originate from opposite ends of the system), $\mu_1$ and $\mu_2$ respectively, and the zero temperature net current is given by $I = (e/\hbar)(\mu_1 - \mu_2)$. The respective conductance is $G = I/V = I/[(\mu_1 - \mu_2)/e] = e^2/\hbar$. At finite temperature the bands are populated according

---

Figure 2. (a) Schematic diagram of a perfect ring with $N$ sites, where the sites are numbered in an anti-clockwise way, threaded by magnetic flux $\Phi$. (b) Energy spectra of the ring with 12 sites with and without magnetic flux. The flux shifts the energy dispersion curve.
to the Fermi–Dirac distribution \( f(\epsilon, \mu) = \frac{1}{1 + \exp[(\epsilon - \mu)/k_BT]} + 1 = f_0(\epsilon - \mu) \) and 
the current becomes \( I = (e/h) \int_{-\infty}^{\infty} f_0(\epsilon - \mu_1) - f_0(\epsilon - \mu_2) \). The final ingredient is 
the introduction of an obstacle (a structural or potential barrier) in the path of the 1D electrons. An 
electron with energy \( \epsilon \) is transmitted through the barrier with probability \( |t(\epsilon)|^2 \), as explained 
above, and the current becomes \( I = (e/h) \int_{-\infty}^{\infty} |t(\epsilon)|^2 [f_0(\epsilon - \mu_1) - f_0(\epsilon - \mu_2)] \). Since 
\( \mu_1 - \mu_2 = eV \), the differential conductance \( G = dI/dV \) for spinless fermions on the lattice is 
given by 
\[
G(T) = \frac{\pi^2 k_B^2}{h^2} \int_{-\infty}^{\infty} \left(-\frac{df}{d\epsilon}\right) |t(\epsilon)|^2 \, d\epsilon, 
\]
(8)
where \( f = f(\epsilon, \mu) \) is the Fermi–Dirac distribution [14]. For zero temperature, \( G(0) = \frac{\pi^2}{2} |t(\mu)|^2 \). The energy interval of integration corresponds to the energies of the one-particle 
eigenstates of the 1D tight-binding leads with hopping integral \( t = 1 \), since for time much 
earlier or later than when the incident wave packet is in the neighborhood of the cluster, the 
particle can be described as a 1D tight-binding particle. That is, the energy spectra (and also 
itse density of states) for extended states in the system of coupled leads and cluster remains the 
same as for the leads without coupling to the cluster.

The hoppings \( t_L \) and \( t_R \) generate finite transmission probability across the cluster. Since 
no two-particle interactions are considered in this paper, the transmission probability \( |t(\epsilon_i)|^2 \) 
for an incident particle with momentum \( \kappa \) and energy \( \epsilon_i = -2\cos(k) \) can be calculated, 
solving directly the respective eigenvector equation for the tight-binding Hamiltonian, 
\( \hat{H} |\Psi_k\rangle = \epsilon_k |\Psi_k\rangle \). This method is similar to that followed in the determination of the band 
structure of a tight-binding model, which is usually taught in an undergraduate solid state 
course. Since \( |\Psi_k\rangle = \sum_{n=0}^{\infty} \psi_n |n\rangle \), where \( \psi_n \) is the eigenfunction amplitude at site \( n \), the 
eigenvector equation can be written as a matrix equation \( [\hat{H}] |\psi\rangle = \epsilon_k |\psi\rangle \), where \( |\psi\rangle \) is the 
column vector of the eigenfunction amplitudes \( \psi_n \) and \([\hat{H}] \) is the matrix representation of the 
Hamiltonian in the Wannier function basis \([|n\rangle]\). This matrix equation is equivalent to an 
infinite system of linear equations (the number of equations is equal to the number of sites 
which is infinite in our system) of the form 
\[
\epsilon_k \psi_n = \sum_{m=\infty}^{\infty} H_{nm} \psi_m, 
\]
(9)
where \( H_{nm} = \langle n|\hat{H}|m\rangle \). The matrix element \( H_{nm} \) is zero except if the site \( m \) is a nearest neighbor 
of site \( n \) or if \( m = n \). One should now recall that our system is constituted by the left lead, the 
cluster and the right lead. If \( t_L = t_R = 0 \), the system of equations decouples into three 
independent sets of equations and the particle can be restricted to one of the three regions. 
For instance, the eigenvectors and eigenvalues when the particle is confined to the cluster are 
obtained from \( [\hat{H}_c] |\psi_5\rangle = \epsilon |\psi_5\rangle \), where \( |\psi_5\rangle \) is the column vector of the eigenfunction 
amplitudes at the cluster sites and the corresponding equations in the case of the tight-binding 
ring are of the form 
\[
\epsilon \psi_j = \epsilon_j \psi_j - te^{i\theta}/N \psi_{j+1} - te^{-i\theta}/N \psi_{j-1}, 
\]
(10)
where \( j = 1, \ldots, N \) and with periodic boundary conditions, \( \psi_{N+1} = \psi_1 \).

Let us now assume finite \( t_L \) and \( t_R \). Since we are interested in the transmission probability 
of a right-moving particle, we can limit our study to states with energy \( \epsilon_i = -2\cos(k) \), which 
can be written as an incident wave plus the respective reflected wave on the left lead and 
a transmitted wave on the right lead. This implies that the equations for the wavefunction 
amplitude at any site \( j \) of the leads (with \( j < 0 \) or \( j > N + 1 \)), 
\[
\epsilon_k \psi_j = -\psi_{j+1} - \psi_{j-1}, 
\]
(11)
4. Results

We have applied the method described in the previous section to the determination of the differential conductance of an open tight-binding ring under electric field and threaded by magnetic flux. We also look into the effect of reducing one of the hopping integrals in the ring, effectively changing the boundary conditions from periodic to open. We also consider the influence of the radial electric field created by a charged impurity in the neighborhood of the ring and the results obtained lead us to suggest that conductance through clusters may be used as a new tool for microscopy, that is, its sensitivity to local electric fields can, in principle, be used to obtain images in a similar way as for a scanning tunneling microscope.

In order to better understand the results for the conductance, the energy spectrum of the isolated ring is determined. In the center plot of figure 3(d), we show the energy spectrum of a ring with eight sites as a function of the magnetic flux with \( \epsilon_i = 0 \) and nearest-neighbor hopping \( t = 1 \), see figure 3(b). This energy spectrum follows the behavior described by equation (7).
Figure 3. Schematic representation of a ring with eight sites: (a) in the presence of an in-plane uniform electric field ($eE_y = 0.5$); (b) in the absence of an electric field; and (c) with one of the hopping integrals, $t_1$, equal to zero. The contact sites to the leads are indicated in red. (d) Respective plots of the energy levels and conductance as functions of the normalized magnetic flux $\Phi/\Phi_0$. The conductance is evaluated for two values of chemical potential, $\mu = 0.01$ and 1. Red and blue dashed lines indicate these values of energy in the top plots. In the center plot, the Aharonov–Bohm effect in the conductance with a half quantum flux periodicity is observed, as well as zero conductance for $\Phi/\Phi_0 = n + 1/2$ (reflecting the destructive interference of the plane waves traveling through the two branches of the ring). The Aharonov–Bohm effect disappears in the broken ring, as expected.

Exactly. The left plot displays the same spectrum when a planar uniform electric field is present, $eE_y = 0.5$, see figure 3(a). This planar electric field shifts the on-site energy of every site, $\epsilon_j \rightarrow \epsilon_j + e\vec{r}_j \cdot \vec{E}$. The right plot corresponds to the change of boundary conditions from periodic to open, see figure 3(c). In the left and center plots, the Aharonov–Bohm oscillations of the ground state energy are observed, while in the right plot they are absent. The application of the electric field leads to two changes in the energy spectra. (i) The perturbation caused by the electric field has a first order effect for degenerated states and a second order effect for non-degenerate levels. This means that a perturbation produces a ‘repulsion’ between levels
that is stronger the closer the levels are. (ii) The influence of the magnetic field decreases as the electric field intensity increases. For high enough values of electric field the energy oscillations due to the magnetic flux are no longer present and the energy dependence on flux becomes flat, reflecting the localization of the particles due to the large differences between on-site energies.

The respective plots of the conductance, evaluated at two values of chemical potential, \( \mu = 0.01 \) and 1 (which are indicated by red and blue dashed lines in the top plots) are shown in the bottom plots of figure 3(d). In the center plot, the Aharonov–Bohm effect in the conductance with a periodicity of one quantum flux is observed, as well as zero conductance for \( \Phi / \Phi_0 = n + 1/2 \), with integer \( n \) (reflecting the destructive interference of the plane waves traveling through the two branches of the ring). The Aharonov–Bohm effect disappears in the broken ring. The conductance has peaks when the chemical potential has the same value as any of the system eigenvalues. This is called resonant tunneling and for weak coupling to the leads, these peaks have the Breit–Wigner shape [3, 15]. Note that the conductance profiles are very sensitive to changes in the chemical potential.

Now, we discuss the influence of non-uniform local electric fields in the conductance through the ring. In the following, we consider a radial electric field generated by a charged impurity in the proximity of the ring, according to the Coulomb’s law, but other forms of local electric fields should lead to similar results. We neglect the possibility of particle hoppings between the cluster and the impurity, as well as the effect of the electric field in the leads. As in the case of the uniform electric field, this field changes the on-site energy, which is now given by \( \epsilon_j \rightarrow \epsilon_j + \frac{C}{|r_j - r|} \), where \( C \) is a constant. The impurity is kept at a fixed distance \( z \) of the ring plane (this distance acts as a cutoff to the Coulomb potential) and its position is swept in the \( x \) and \( y \) direction, the conductance being calculated for each impurity position. The respective contour plots are shown in figure 4, for the three cases described by figures 3(a)–(c), namely, figures 4(a)–(c) in the case of the perfect ring, figures 4(d)–(f) in the case of the ring with an applied electric field and figures 4(g)–(i) in the case of the broken ring. In general, we observe in these contour plots, peaks or dips in the conductance when the impurity \((x, y)\) position coincides with a site of the ring. In the case of figures 4(a)–(c) (perfect ring), depending on the value of the chemical potential, peaks or dips appear with a symmetric configuration, which reflects two factors: (i) the probability density of the eigenstates of the ring Hamiltonian and in particular of the eigenstate with energy nearest to the chemical potential; (ii) the influence of the leads, which effectively changes the on-site energy of the two contact sites of the ring. Qualitatively, one may say that the leads lift the degeneracy of the energy spectra of the ring and since this effect is local, the standing waves in the ring with the same momentum acquire different energies (the difference is small for weak coupling to the leads). Therefore, one can infer the probability density of these standing waves from the conductance contour plots in the case of the symmetric ring.

When an electric field is applied, the eigenstates of the ring have less symmetrical probability density profiles, with more probability density being accumulated in the ring in the direction of the electric field or in the opposite direction, depending on the energy of the eigenstate. This is reflected by the conductance contour plots of figures 4(d)–(f), where the lessening of symmetry is observed. Note that for fixed chemical potential, varying the electric field, the energy of the eigenstates of the ring is increased and several crossings of the eigenvalues of the ring with chemical potential occur, as shown in figure 3(d), so that in the conductance contour plots, probability density distributions corresponding to different eigenstates of the ring are observed. Breaking a hopping link in the tight-binding ring has an even stronger effect in the eigenstate probability densities of the ring. In figures 4(g)–(i), the absence of symmetry is clearly observed. Again, adjusting the chemical potential, the
conductance of the broken ring become more sensitive to local electric fields in different regions of the \( xy \) plane.

The sensitivity to local electric fields, as well as the possibility of probing different points of space adjusting the chemical potential, leads us to suggest that conductance through clusters may be used as a new tool for microscopy, that is, it can, in principle, be used to obtain images in a similar way as for scanning tunneling microscope. Note that small changes in the vertical position of the impurity do not change the conductance shape significantly. The farther the impurity is from the cluster plane, the less it couples to the cluster and the smoother the conductance plot becomes.

5. Conclusion

In this paper, we showed how to determine numerically the effects of applied magnetic and electric fields on the conductance of tight-binding quantum clusters connected to
one-dimensional leads, using a simple tight-binding method which could be programmed by an undergraduate student attending a solid state course or a final-year project. Important phenomena of transport through nanorings, such as Aharonov–Bohm conductance oscillations, resonant tunneling and destructive interference are observed as the magnetic field, chemical potential and other parameters are varied. We have explored in particular the effect of a charged impurity on the conductance through the ring. We observed that the conductance has a strong sensitivity to the local electric field and suggested that it can, in principle, be used to obtain images in a similar way as for scanning tunneling microscope.

Acknowledgments

AAL was supported by Fundação para a Ciência e a Tecnologia (Portugal), co-financed by FSE/POPH, under grant SFRH/BD/68867/2010.

References

[1] Gorter C J 1951 A possible explanation of the increase of the electrical resistance of thin metal films at low temperatures and small field strengths Physica 17 777–80
[2] van Wees B J, van Houten H, Beenakker C W J, Williamson J G, Kouwenhoven L P, van der Marel D and Foxon C T 1988 Quantized conductance of point contacts in a two-dimensional electron gas Phys. Rev. Lett. 60 848–50
[3] Douglas Stone A and Lee P A 1985 Effect of inelastic processes on resonant tunneling in one dimension Phys. Rev. Lett. 54 1196–9
[4] Aharonov Y and Bohm D 1959 Significance of electromagnetic potentials in the quantum theory Phys. Rev. 115 485–91
[5] Webb R A, Washburn S, Unbach C P and Laibowitz R B 1985 Observation of $\pi$ Aharonov–Bohm oscillations in normal-metal rings Phys. Rev. Lett. 54 2696–9
[6] Marder M P 2010 Condensed Matter Physics (New York: Wiley)
[7] Li J, Zhang Z-Q and Liu Y 1997 Resonant transport properties of tight-binding mesoscopic rings Phys. Rev. B 55 5337–43
[8] Koval D, Sivan U, Entin-Wohlman O and Imry Y 1990 Transmission through multiply-connected wire systems Phys. Rev. B 42 9009–18
[9] Orellana P A, Ladrón de Guevara M L, Pacheco M and Latgé A 2003 Conductance and persistent current of a quantum ring coupled to a quantum wire under external fields Phys. Rev. B 68 195321
[10] Datta S 2005 Quantum Transport: Atom to Transistor 2nd edn (Cambridge: Cambridge University Press)
[11] Meir Y and Wingreen N S 1992 Landauer formula for the current through an interacting electron region Phys. Rev. Lett. 68 2512–5
[12] Taylor J R 1972 Scattering Theory: The Quantum Theory on Nonrelativistic Collisions (New York: Wiley)
[13] Enss T, Meden V, Andergassen S, Barnabé-Thiriault X, Metzner W and Schönhammer K 2005 Impurity and correlation effects on transport in one-dimensional quantum wires Phys. Rev. B 71 155401
[14] Landauer Rolf 1970 Electrical resistance of disordered one-dimensional lattices Phil. Mag. 21 863–7
[15] Breit G and Wigner E 1936 Capture of slow neutrons Phys. Rev. 49 519–31