

The Aharonov-Bohm Effect and Persistent Currents in Quantum Rings

Alexandre Miguel de Araújo Lopes

Department of Physics
University of Aveiro

Advised by:
Ricardo A. G. Dias

2007/2008

Preface

When I first started this thesis I hadn't had a solid state physics subject yet and therefore I had to acquire some basic knowledge before dedicating myself to this thesis. After some initial hickups, I think things worked out well and I certainly did learn a lot along the road.

Throughout this thesis I tried to stick with S.I. units. Though most of the documentation that can be found on the subjects studied in this thesis are written in C.G.S units, and although I think that C.G.S units do make Maxwell's equations look extremely beautiful and simple, I didn't find any advantage in using them over the S.I. units in this case.

The *Mathematica* notebooks used for the numerical calculations in this thesis can be found at <http://www.quantumrings.vndv.com/>.

I would like to express my thanks to those persons who always stood there for me: my parents, my brother and Filipa - a big thanks to all of you. I would also like to thank Daniel Gouveia, my colleague and friend, for all the conversations that we had which have inspired me. To LÍdia del Rio, who always cheered up the time we spent at our advisor's office by talking about really non sense stuff and fun comics. And finally I would like to thank my advisor, Ricardo Dias, for all the knowledge I have acquired from him and because without him this thesis would simply not exist.

Contents

1	Introduction	4
1.1	Objectives	4
1.2	Persistent currents	4
1.3	Aharonov-Bohm effect	5
2	Ring models	6
2.1	Introducing ring models	6
2.2	Free electron gas model	6
2.3	Tight-binding model	7
2.4	Interacting spinless fermions	7
3	Free electrons in a ring	8
3.1	Flux dependence of the energy and magnetic moment levels	8
3.2	Persistent currents	10
4	Tight-binding perfect ring	13
4.1	Tight-binding Hamiltonian	13
4.2	Persistent currents	15
5	Disorder effects	16
5.1	One impurity ring	16
5.2	Disordered ring	18
6	Interacting spinless fermions	20
6.1	The strong coupling limit	20
6.2	Currents from different subspaces	20
6.3	t-V ring with an impurity	21
A	Electromagnetic Hamiltonian	24
B	Second quantization Fermionic operators	25
C	Electrical current operator	26
C.1	Free electron gas	26
C.2	Tight-binding model	26
D	Wavefunctions for a free electron in a ring	28

E	Free electron persistent current calculation	29
F	Tb Hamiltonian with external magnetic flux	31

Chapter 1

Introduction

1.1 Objectives

This thesis objective is to study, theoretically, some properties of quantum rings enclosing an external magnetic flux, namely persistent currents, using different models. We will first study independent electrons via the free electron gas model and the tight-binding model, and finally we will address correlated electrons by studying the t-V model, which is basically an extension of the tight-binding model. To achieve the objectives of this thesis, analytical and numerical calculations were performed. The numerical calculations they were done using *Mathematica* and the notebooks can be found at <http://www.quantumrings.vndv.com/>.

1.2 Persistent currents

Persistent currents are currents (i.e. charge movement) which are able to sustain themselves independently from an applied voltage difference. Persistent currents have been long known and studied in superconductors. In quantum rings, we can have same persistent currents too despite their origin being different. Theoretically, persistent currents in quantum rings have been known for some time [1, 2] and they have also been measured experimentally using SQUIDS [3].

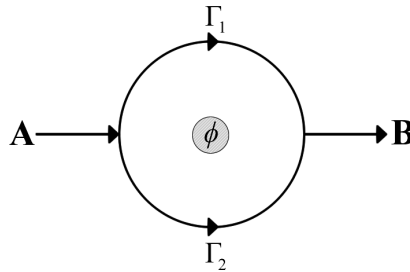


Figure 1.1: Aharonov-Bohm effect general geometry.

1.3 Aharonov-Bohm effect

The Aharonov-Bohm effect [4] is a quantum mechanical effect that results from gauge invariance. It states that if we have electrons travelling along two paths and if between those paths there is a magnetic flux which vanishes in the region where the electrons flow (i.e. there is no magnetic force acting on the travelling electrons), this same magnetic flux will produce a phase shift in the electrons' wavefunction (Fig. 1.1). Assuming that the paths are equal, Aharonov-Bohm effect results in a phase shift given by,

$$\Delta\varphi = \frac{q}{\hbar} \oint_C \vec{A} \cdot d\vec{l}, \quad (1.1)$$

where $\vec{A}$ is the vector magnetic potential.

Chapter 2

Ring models

2.1 Introducing ring models

There are several models in solid state physics which can be used to treat the problem of electrons in a ring. Here we will address this problem using models of increasing complexity starting with non-correlated models and considering a perfect ring and finally we will address disorder and correlated electrons. We will address the problem of electrons in a ring using the free electron gas and the tight-binding models, for the non correlated case, and the t-V model for the correlated case. All these models are used for spinless fermions (although the tight binding model can be used for fermions with spin). The Hubbard model is a popular model which takes spin and Coulomb on-site interaction in account but we will not use it here.

2.2 Free electron gas model

The free electron gas model was one of the first models used in solid state physics. It is an oversimplified model and that should not be forgotten when working with it. Nevertheless it is simple to solve analytically and it can prove extremely useful as a first approach to a problem. Electron gas model assumes that electrons behave much like a classical ideal gas. It assumes that electrons are independent, i.e., the Coulomb interaction between them is assumed to be zero, and free, i.e., they don't feel a periodic potential from ions (only a global potential which prevents the electrons from leaving the solid). Using this approach we can treat every electron separately, using the free electron Hamiltonian¹:

$$H = \frac{(\vec{p} - q\vec{A})^2}{2m}, \quad (2.1)$$

where $\vec{p}$ is the conjugate momentum, $\vec{A}$ is the magnetic vector potential and q and m are the particle's charge and mass respectively.

¹See Appendix A for the Hamiltonian's derivation.

2.3 Tight-binding model

The tight-binding model assumes that the Hamiltonian close to a lattice point can be approximated by the Hamiltonian of an isolated atom centered at that lattice point [5]. This way an electron's wavefunction in a one-dimensional crystal can be written as a linear combination of the electron's wavefunctions in the sites, that is,²

$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_{j=1}^N e^{ikj} c_j^\dagger |0\rangle, \quad (2.2)$$

where N is the number of sites, k the momentum and $c_j^\dagger$ the fermionic creation operator.³ In second quantized form, the tight-binding Hamiltonian in a linear 1-D system can be written as a "hopping" Hamiltonian,

$$H = -t \sum_{j=1}^N \left[c_j^\dagger c_{j+1} + h.c. \right], \quad (2.3)$$

where t is the one of the band theory overlap integrals [5]. Here we will call t the *hopping factor*.

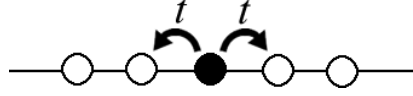


Figure 2.1: The tight-binding model (in second quantized form) assumes that an electron can "hop" to its nearest neighbors if they are not occupied by an electron of the same spin.

2.4 Interacting spinless fermions

In order to address correlations between electrons due to the Coulomb interactions we are going to study interacting spinless fermions using the t-V model. The t-V model is an extended version of the tight-binding model which takes in account the Coulomb interaction between nearest neighbors. Spin is not considered in this model as a simplification. Overall this is a decent model to apply in case we have a rather strong external magnetic field that aligns the system's spins in which case, neglecting spin-spin interactions is the same as having no spin. The Hamiltonian of the t-V model in second quantized form is written as:

$$H = -t \sum_{j=1}^N \left[c_j^\dagger c_{j+1} + h.c. \right] + V \sum_{j=1}^N n_j n_{j+1}. \quad (2.4)$$

where V is the Coulomb energy between two nearest-neighbors electrons and $n_j = c_j^\dagger c_j$ is the occupation number at site j .

²See Appendix B if you are unfamiliar with second quantization.

³Note that the lattice constant was chosen to be equal to 1. This is a usual convention in theoretical solid state physics and is used throughout this thesis.

Chapter 3

Free electrons in a ring

In this chapter we will address a continuous ring using the free electron gas model. After calculating some electronic properties of the system we will introduce a weak potential and calculate the same properties again, comparing the differences between the system with and without the weak potential.

3.1 Flux dependence of the energy and magnetic moment levels

Considering the Schrödinger's equation for a free electron in a ring,

$$\frac{\left(-i\hbar\vec{\nabla}_{polar} + e\vec{A}\right)^2}{2m}\psi = E\psi, \quad (3.1)$$

where ∇_{polar}^2 is the del operator in polar coordinates, we easily arrive at the electron's wavefunction,¹

$$\psi_n(\theta) = \frac{1}{\sqrt{2\pi R}}e^{in\theta}, \quad (3.2)$$

where R is the ring radius, θ the angular position on the ring (see Fig. 3.1) and n a quantum number.

Operating with the free electron's Hamiltonian (2.1), $H\psi_n = E_n\psi_n$, we arrive at an expression for E_n ,

$$E_n = \frac{\hbar^2}{2mR^2} \left(n + \frac{RAe}{\hbar}\right)^2, n = 0, \pm 1, \pm 2, \dots \quad (3.3)$$

Considering a non vanishing magnetic field, enclosed by the ring, concentric with it and having polar symmetry, we get, by applying Stokes' theorem, $\phi = 2\pi AR$, where A is the intensity of the vector magnetic potential in the ring. By defining the quantum of flux as $\phi_o = h/e$ we can write

$$E_n = E_0 \left(n + \frac{\phi}{\phi_o}\right)^2, n = 0, \pm 1, \pm 2, \dots \quad (3.4)$$

¹see Appendix D for a deduction of this wavefunction.

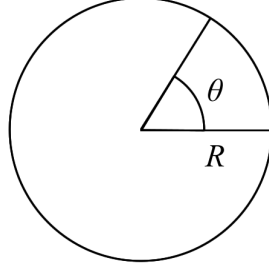


Figure 3.1: Figure showing the coordinates used.

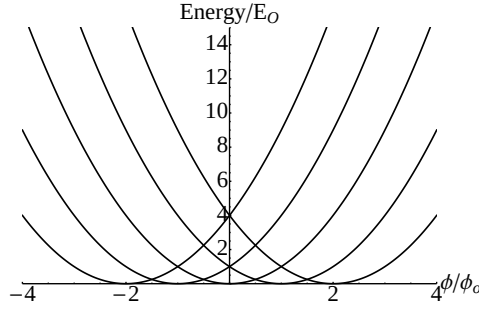


Figure 3.2: Energy dependence on the quantum of flux for the first five levels. Note that for $\phi = 0$ the eigenvalues are doubly degenerate, except for $n = 0$.

where $E_0 = \frac{\hbar^2}{2mR^2}$.

By analysis of Eq. (3.4) we can see that its graphics (see Fig. 3.2) are parabolas. The parabolas with vertices located to the left of the energy axis correspond to positive values of n and the parabolas with vertices is located to the right of the energy axis correspond to negatives values of n . The points where different parabolas meet are points of degeneracy.

Knowing that the magnetic moment is given by [6]

$$M = -\frac{\partial E}{\partial B}, \quad (3.5)$$

and assuming that $\vec{B}$ is constant, we can write the electron's magnetic moment as

$$M_n = -M_0 \left(n + \frac{\phi}{\phi_0} \right), \quad (3.6)$$

where $M_0 = \frac{e\hbar}{2m}$.

By using a numerical approach in *Mathematica* we studied the effect of inserting an arbitrary weak potential in the free electron's Hamiltonian (Eq. (2.1)). The results obtained (figures 3.4 and 3.5) reveal periodicity in the flux for the energy and for the magnetization, due to Aharonov-Bohm effect as we would expect. Note that the periodicity can only be seen in the middle of the figure due to the fact that we have only calculated the energy for the first five levels. By using a hypothetical infinite number of levels we could see the full periodicity.

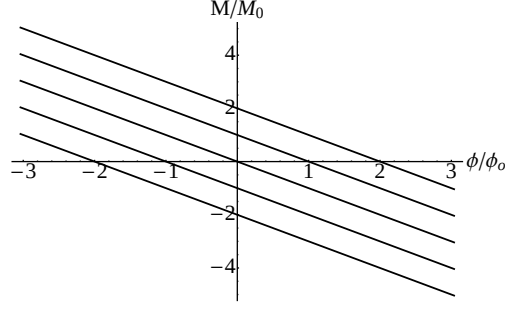


Figure 3.3: Magnetization dependence on the magnetic flux for the first five levels

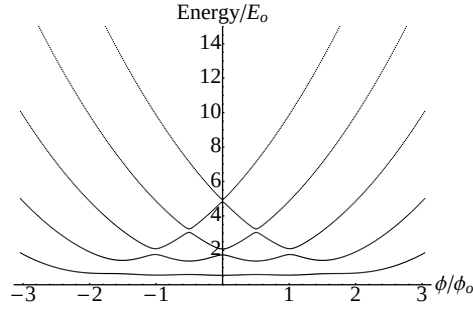


Figure 3.4: Energy dependence on the magnetic flux for the first five levels in the presence of a weak potential.

3.2 Persistent currents

Knowing that the electric current per energetic level is given by ²

$$I_n = -\frac{\partial E_n}{\partial \phi}, \quad (3.7)$$

we can calculate the system's current by summing over all occupied levels. The current of the fundamental state for a system with N_e electrons is then,

$$I_{Total}(\phi) = -I_o'' \sum_{n=n'_F}^{n_F} \left(n + \frac{\phi}{\phi_o} \right). \quad (3.8)$$

where n'_F is the Fermi number for the negative levels, i.e. the smallest level occupied, n_F is the Fermi number for positive levels, i.e. the largest level occupied and $I_o'' = \frac{he}{mL}$ is a constant.

In order to know which levels are occupied we will limit our study to the zero temperature case. We have to take in account the levels occupancy in order to calculate the total current (this can be seen by a careful analysis of Fig. 3.2). After performing some calculations³ we arrive at the following expression for $I_{Total}(\phi)$ in the interval $\in [-0.5\phi_o, 0.5\phi_o]$,

²See Appendix C for a deduction of this formula.

³See Appendix E.

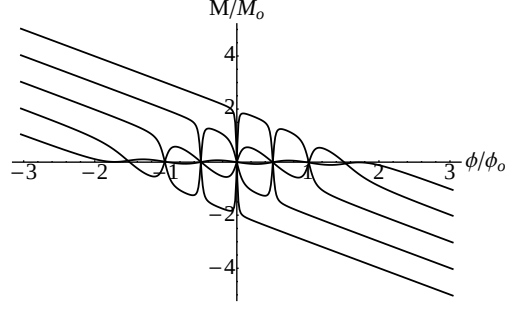


Figure 3.5: Magnetization dependence on the magnetic flux for the first five levels in the presence of a weak potential normalized to the zero potential case.

$$I_{Total}(\phi) = \begin{cases} -I_o \frac{2\phi}{\phi_o}, & N_e \text{ odd}, \frac{\phi}{\phi_o} \in [-0.5, 0.5[\\ -I'_o \left(\frac{2\phi}{\phi_o} + 1 \right), & N_e \text{ even}, \frac{\phi}{\phi_o} \in [-0.5, 0[\\ -I'_o \left(\frac{2\phi}{\phi_o} - 1 \right), & N_e \text{ even}, \frac{\phi}{\phi_o} \in]0, 0.5[\end{cases} \quad (3.9)$$

where

$$I_o = \frac{\hbar e}{mL} \left(n + \frac{1}{2} \right), \quad (3.10)$$

and

$$I'_o = \frac{\hbar e}{mL} (n + 1). \quad (3.11)$$

For a fairly large n_F , i.e., for a large number of electrons, we have that $I_o \approx I'_o$ and in this case we obtain the results displayed on Fig. 3.6a and Fig. 3.6b. The persistent currents are periodic in the magnetic flux with period ϕ_o .

If we consider an ensemble of quantum rings with a uniform N_e distribution in a certain interval such that, half the rings have an even number of electrons and half the rings have an odd number of electrons, then, averaging the persistent current in this case results in a period which is *half* the period for a single ring and we get a decrease in the amplitude by *half* too as seen in Fig. 3.6c.

To summarize, the Aharonov-Bohm effect tends to make the ring's thermodynamical properties periodic in the flux. In the particular case of persistent currents we showed that they are dependent on the parity of the number of electrons. We have also demonstrated that the effect of averaging the persistent currents over an ensemble of rings with an uniform distribution of the number of electrons in a certain interval, is a halving of the periodicity and of the amplitude of the persistent current when compared to that of a single ring. These results agree with experimentally obtained ones. [7, 8].

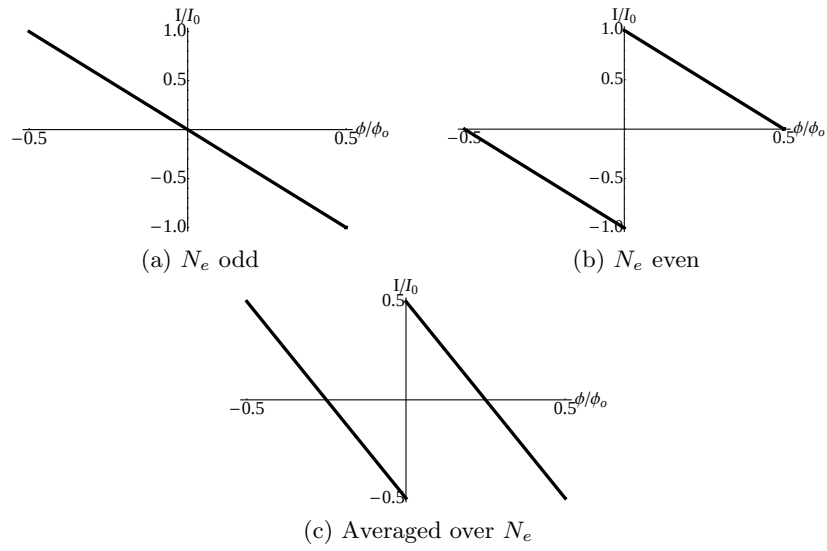


Figure 3.6: As we can clearly see the persistent currents for an even and an odd number of electrons are different but both have the same periodicity. We can also see that averaging the persistent currents over N_e results in a halving of the period and of the maximum current when compared to a single ring case.

Chapter 4

Tight-binding perfect ring

In this chapter we will address a discrete ring enclosing a magnetic flux, with N identical sites (see Fig. 4.1), using the tight-binding model. The energy, magnetic moment and persistent currents for the system are calculated and analyzed. In a first approach to the problem the magnetic flux is assumed to be zero.

4.1 Tight-binding Hamiltonian

A ring is a 1-D system, linear in polar coordinates, with periodic boundary conditions,

$$|N + 1\rangle = |1\rangle, \quad (4.1)$$

which results in momentum's quantization,

$$k = \frac{2\pi m}{N}, \quad m = 0, 1, 2, \dots, N - 1. \quad (4.2)$$

Applying the tight-binding Hamiltonian [Eq. (2.2)] over the electron wavefunction [Eq. (2.3)] and inserting the ring's periodic boundary conditions we obtain the eigenvalues of the Hamiltonian,

$$\begin{aligned} E &= -2t \cos(k) \\ &= -2t \cos\left(\frac{2\pi n}{N}\right), \quad n = 0, 1, 2, \dots, N - 1. \end{aligned} \quad (4.3)$$

We can also define the energy such that the electron wave vectors are confined to the first Brillouin zone, [5]

$$\begin{aligned} k(m) &= \frac{2\pi m}{N}, \quad m \in \left[-\frac{N}{2}, \frac{N}{2}\right[\wedge m \in \mathbb{Z} \\ k(m) &\in [-\pi, \pi[, \end{aligned} \quad (4.4)$$

which is usual in solid state physics and allows us to get a better visualization of the energy dispersion relation (see Fig. 4.2a and Fig. 4.2b).

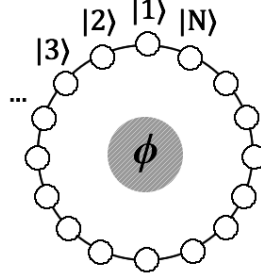


Figure 4.1: A perfect ring with N identical sites surrounding an external magnetic flux.

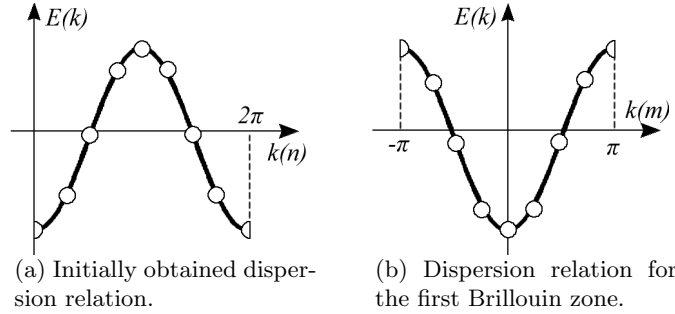


Figure 4.2: Comparison of the plots of the energy dispersion relation for wave vectors lying in the first and the second Brillouin zone and for wave vectors lying only in the first Brillouin zone.

In order to study a ring enclosing an external magnetic flux, an Aharonov-Bohm phase must be introduced in the Hamiltonian. One we must have

$$\psi(2\pi) = e^{i(2\pi\phi/\phi_o)}\psi(0), \quad (4.5)$$

i.e., the electron's wavefunction must shift its phase by $2\pi\phi/\phi_o$, after the electron has completed a loop around the ring.¹ This can be achieved by writing the translational invariant Hamiltonian²

$$H = -t \sum_{j=1}^N \left[e^{i(\phi'/N)} c_j^\dagger c_{j+1} + h.c. \right], \quad (4.6)$$

where $\phi' = 2\pi\phi/\phi_o$ is the reduced flux and $\phi_o = e/h$ is the quantum of flux.

Applying the Hamiltonian to the electron wavefunction [Eq. 2.3] one obtains

$$E = -2t \cos \left(k - \frac{\phi'}{N} \right), \quad (4.7)$$

where k has the same values as before [Eq. (4.4)].

¹This is known as twisted boundary conditions.

²See Appendix F for a deduction of this Hamiltonian.

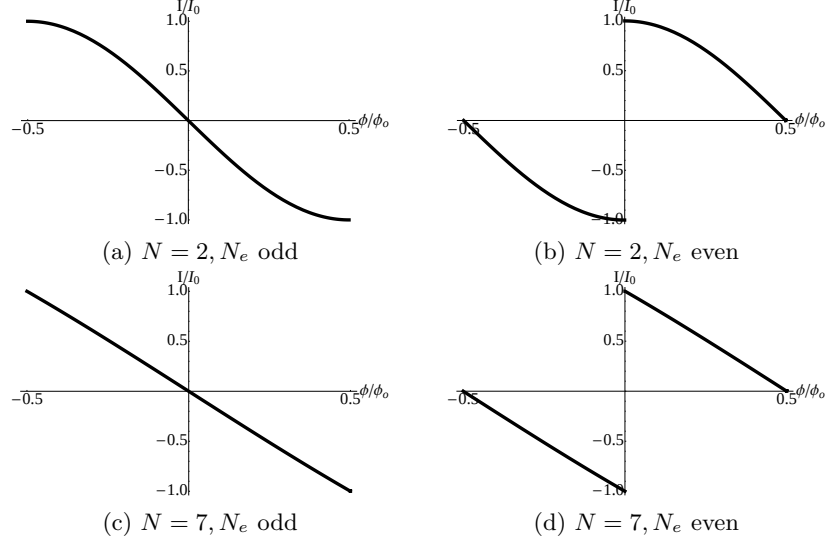


Figure 4.3: Persistent currents for an odd and an even number of electrons.

4.2 Persistent currents

The persistent currents can be calculated in a way similar to the free electron case using Eq. (3.7),³ which for the tight-binding model leads to,

$$I_{Total}(\phi) = \begin{cases} -I_o \frac{\sin(2\pi/N\phi/\phi_o)}{\sin(\pi/N)}, & N_e \text{ odd}, \frac{\phi}{\phi_o} \in [-0.5, 0.5[\\ -I_o' \frac{\sin(\pi/N(2\phi/\phi_o + 1))}{\sin(\pi/N)}, & N_e \text{ even}, \frac{\phi}{\phi_o} \in [-0.5, 0[\\ -I_o' \frac{\sin(\pi/N(2\phi/\phi_o - 1))}{\sin(\pi/N)}, & N_e \text{ even}, \frac{\phi}{\phi_o} \in]0, 0.5[\end{cases} \quad (4.8)$$

One can see that the persistent current is, like in the free electron gas, different for an even and an odd number of electrons (Fig. 4.3a and 4.3b). We can also see that for $N \gtrsim 7$ the persistent currents for the tight-binding model and for the free electron gas model are practically identical (Fig 4.3c and 4.3d).

As was expected, the persistent currents in the tight-binding model are periodic in the magnetic flux. These persistent currents rapidly approach the results obtained using the free electron gas with increasing number of sites, which is surprising because the tight-binding model is on the other extreme of the free electron gas model.⁴

³see Appendix C for a deduction of this formula for the tight-binding model

⁴That is, in the tight-binding model electrons are assumed to be tightly bound to the ions while in the free electron gas model, electrons are completely free from the ions.

Chapter 5

Disorder effects

Disorder breaks translational invariance making disordered situations harder to study than perfect situations. Nevertheless disorder is responsible for some interesting phenomena in solid state physics [5].

In this chapter disorder is treated for a discrete ring, enclosing a magnetic flux, using the tight-binding model.

5.1 One impurity ring

In a ring with a single impurity the hopping factor from and to the impurity and its on-site energy will differ from the other sites. If we introduce an external flux, we can write the following Hamiltonian for a ring with N sites and an impurity at site N enclosing an external magnetic flux,

$$\begin{aligned}
 H = & \varepsilon_0 \sum_{j=1}^N c_j^\dagger c_j - t \sum_{j=1}^{N-2} \left[e^{i(\phi'/N)} c_j^\dagger c_{j+1} + h.c. \right] \\
 & + \varepsilon_N c_N^\dagger c_N - t_N \sum_{j'=N-1}^N \left[e^{i(\phi'/N)} c_{j'}^\dagger c_{j'+1} + h.c. \right],
 \end{aligned} \tag{5.1}$$

where ε_N is the on-site energy of the impurity, ε_0 the on-site energy of the other sites, t_N is the hopping factor from and to the impurity and t is the hopping factor between non-impurity sites.

The Hamiltonian can be written as $H = H_0 + H'$, where

$$H_0 = \varepsilon_0 \sum_{j=1}^N c_j^\dagger c_j - t \sum_{j=1}^N \left[e^{i(\phi'/N)} c_j^\dagger c_{j+1} + h.c. \right], \tag{5.2}$$

is the perfect ring's Hamiltonian (with translational invariance) and

$$H' = (t - t_N) \sum_{j'=N-1}^N \left[e^{i(\phi'/N)} c_{j'}^\dagger c_{j'+1} + h.c. \right] + (\varepsilon_N - \varepsilon) c_N^\dagger c_N. \tag{5.3}$$

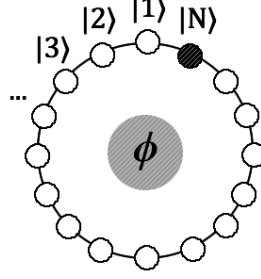


Figure 5.1: A ring enclosing an external flux with an impurity at site N.

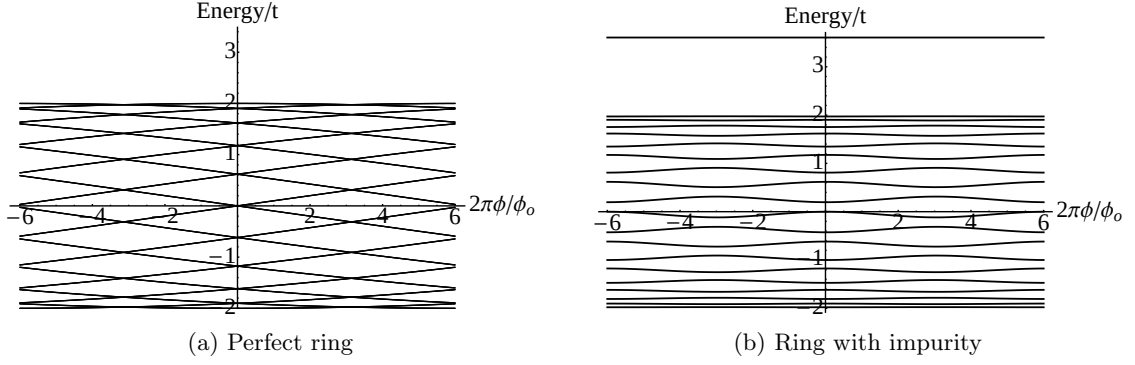


Figure 5.2: Energy vs magnetic flux plot for a perfect ring and for a ring with an impurity with $\varepsilon_0 = 3$ ($N = 20$). It can be seen that we have a state outside the usual energy band (and a lift of the energy degeneracy).

H' can be treated as a perturbative term using first-order time-independent perturbation theory. Doing so one arrives at the eigenvalues of the Hamiltonian, H ,

$$\begin{aligned}
 E &= E_0 + E' = \varepsilon + \frac{1}{N} (\varepsilon - \varepsilon_N) \\
 &\quad - 2t \left(1 - \frac{2}{N}\right) \cos\left(k - \frac{\phi'}{N}\right) - 2\frac{t_N}{N} \cos\left(k - \frac{\phi'}{N}\right) \\
 &= \varepsilon + \frac{1}{N} (\varepsilon - \varepsilon_N) - 2t \cos\left(k - \frac{\phi'}{N}\right) \left(1 - \frac{2}{N} + \frac{t_N}{tN}\right),
 \end{aligned} \tag{5.4}$$

which is the same as for the case of the ring without impurities apart from an additive and a multiplicative constants. Therefore the thermodynamical properties of this system will be very similar to the ones of the ring without impurities.

Let us make in Eq. (5.1), $t = t_N$ and $\varepsilon_N \neq \varepsilon_0$. This case was treated using *Mathematica* and the results obtained were approximately the usual tight-binding energies (with a lift of the energy degeneracy) and a *bound* state which energy lies outside the usual band energy (from $-2t$ to $2t$) as can be seen in Fig. 5.2b. By theory [9] the energy of this state is given by $E = \sqrt{4t^2 + \varepsilon^2}$ which is in agreement with the results obtained.

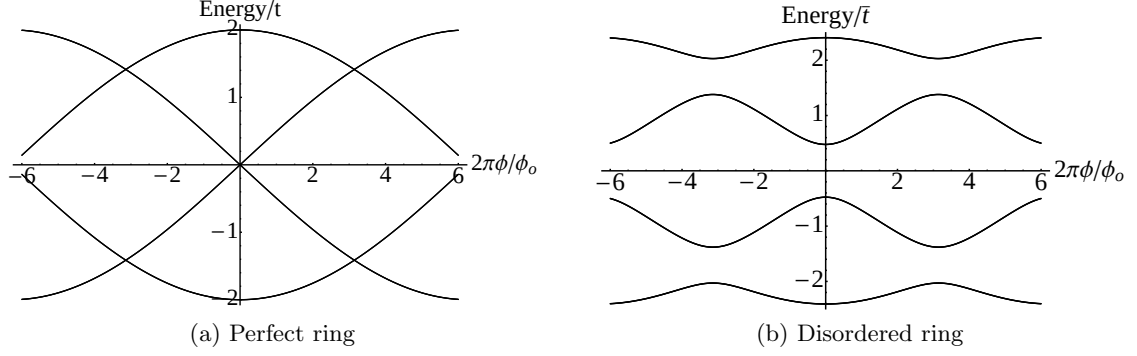


Figure 5.3: Energy vs magnetic flux plot for a perfect ring and a disordered ring with $N = 4$ and t_j chosen randomly (following a normal distribution with average, $\bar{t}$, 2 and standard deviation 0.5). It can be seen that in the disordered ring we have a lift of the energy degeneracy.

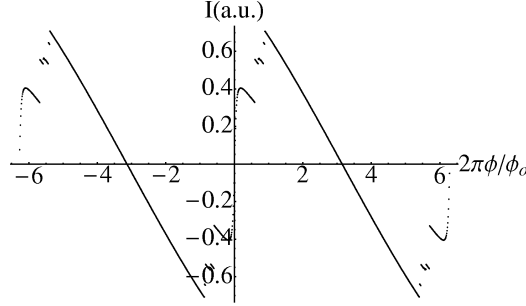


Figure 5.4: Persistent current curves for an ensemble of disordered rings (averaged over 100 disorder configurations). t_j was chosen randomly from a normal distribution with average 2 and standard deviation 0.5 and $\varepsilon_F = -0.8$, $N = 4$. We can see that this plot shows the behaviors expected for a single ring with an even number of electrons and for a single ring with an odd number of electrons.

5.2 Disordered ring

A completely disordered ring can be described by the Hamiltonian,

$$H = \sum_{j=1}^N t_j \left[e^{(i\phi'/N)} c_j^\dagger c_{j+1} + h.c. \right] + \sum_{j=1}^N \varepsilon_j c_j^\dagger c_j, \quad (5.5)$$

with random t_j and/or ε_j .

We addressed the case where $\varepsilon_1 = \varepsilon_2 = \dots$ and t_j were chosen randomly following a normal distribution with average 2 and standard deviation 0.5. For this case the degeneracy in the energy is lifted as can be seen in Fig. 5.3b.

For a given Fermi energy, ε_F , and averaging over a large set of random t_j , one obtains a plot for the averaged persistent currents curves, as shown in Fig. 5.4, where we can see a superposition of the behavior expected for a single ring with an even number of electrons and for a single ring with an odd number of electrons.

As we have shown, the effect of having a single impurity in a ring is rather trivial. The electrons' energy and magnetization are only changed by constants, at least using first order

perturbation theory. On the other hand, if we consider a completely disordered ring, then we see that the degeneracy in the energy is lifted and that if we average over the hopping factor values,¹ then we will see a smoothing of the discontinuities in the system's persistent current.

¹Which can happen if we have an ensemble of rings composed of different impurities.

Chapter 6

Interacting spinless fermions

The t-V model is a spinless tight-binding model where we introduce the Coulomb repulsion between nearest-neighbors fermions.

A general solution for the t-V model is available using the Bethe-ansatz method but this is a non intuitive and extremely difficult method and so we will not make use of it.

6.1 The strong coupling limit

We can, as we did with the tight-binding model, study a ring threaded by an external flux using the t-V model. In order to do this we have to modify our Hamiltonian [Eq. (2.4)], as in the tight-binding case,¹

$$H = -t \sum_{j=1}^N \left[e^{i(\phi'/N)} c_j^\dagger c_{j+1} + h.c. \right] + V \sum_{j=1}^N n_j n_{j+1} \quad (6.1)$$

In the strong coupling limit, $V/t \rightarrow \infty$, the t-V model can be studied without resorting to Bethe-ansatz which makes this situation of particular interest [10]. In this case, the allowed energies will be extremely localized around integer multiples of E/V (see Fig. 6.1). Since $\frac{dE}{d\phi}$ is of the order of t , the persistent currents will be of this order in the strong coupling limit.

Far from the strong-coupling limit the t-V model gets harder to study analytically, but using numerical methods it is easy to see that we have subspaces of energies centered around integer multiples of V as expected (Fig. 6.2). A decrease in the energy periodicity can be observed for some energy levels, namely the "fundamental" level of the top energy subspace.

6.2 Currents from different subspaces

With increasing V it was observed that, for a fixed number of sites N , number of electrons, N_e , and hopping factor, t , the multiparticle persistent currents remains approximately the same for the fundamental level. However for the fundamental level of the top subspace, there is a decrease in its amplitude with increasing V and a change in its shape, which leads to a halving of the periodicity for V higher than a certain value (see Fig. 6.3).

¹see Appendix F for the deduction of the tight-binding Hamiltonian. The deduction of the Hamiltonian for the t-V model is similar.

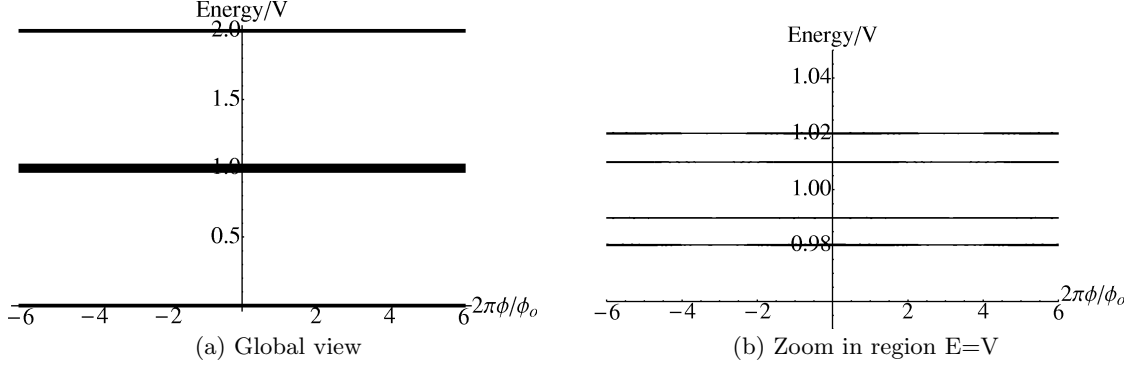


Figure 6.1: Energy-flux plots for a system with $N = 6$ and $N_e = 3$ in the strong coupling limit, $t = 1$, $V = 100$. We can clearly see that we have three allowed values of energy, $E/V \approx 0$, $E/V \approx 1$, $E/V \approx 2$ which are due to the allowed configurations of the system. By zooming in the region we see that for $E \approx V$ we have in fact four allowed values of E as predicted by theory.

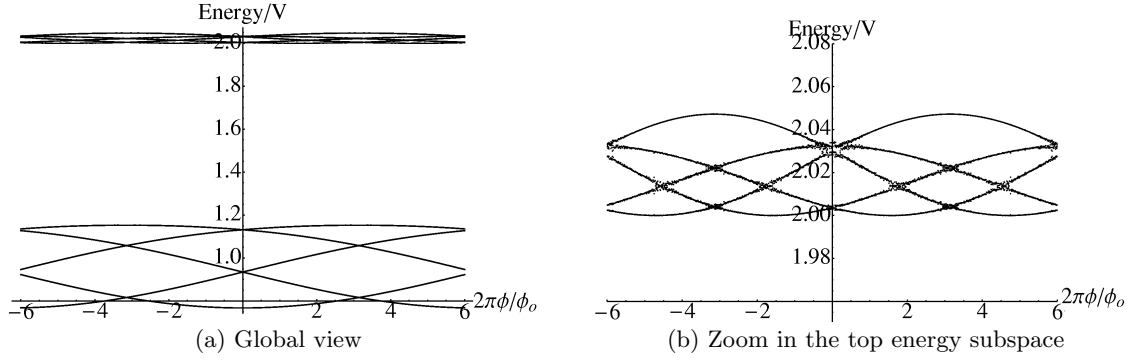


Figure 6.2: Energy plot for a ring with 5 sites and 3 particles treated using the t-V model with $V/t = 10$. On the zoomed region is possible to see that there is a decrease of the period in the lower part.

6.3 t-V ring with an impurity

The Hamiltonian of a t-V ring enclosing a magnetic flux, with an impurity at site N can be written as,

$$\begin{aligned}
 H = & -t \sum_{j=1}^{N-2} \left[e^{i(\phi'/N)} c_j^\dagger c_{j+1} + h.c. \right] \\
 & -t_N \sum_{j=N-1}^N \left[e^{i(\phi'/N)} c_N^\dagger c_{N+1} + h.c. \right] + \varepsilon_N c_N^\dagger c_N + V \sum_{j=1}^N n_j n_{j+1}
 \end{aligned} \tag{6.2}$$

where t_N is the hopping factor to and from the impurity and ε_N is the impurity on-site energy.

We studied the case of inserting an impurity at site N and setting $\varepsilon = 0$. The results obtained show a lift of the energy degeneracy as can be seen in Fig. 6.4.

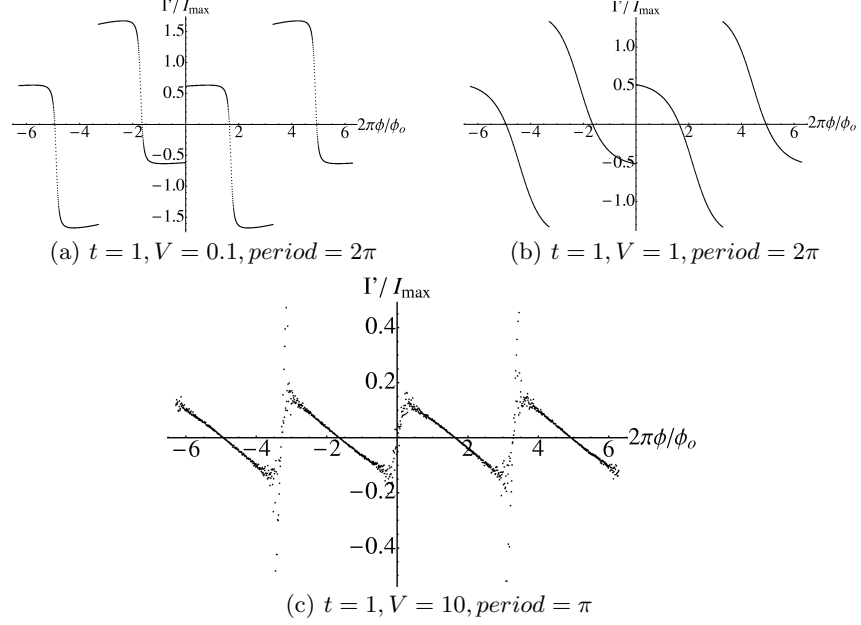


Figure 6.3: Persistent currents for multiple values of V for the fundamental level of the top subspace for a system with $N=5$ and $N_e=3$ ($I_{\max}$ is the maximum value of the persistent current of the fundamental level of the bottom subspace - this value does not change with V). We can see, for the fundamental level of the top energy subspace that the persistent currents shape and amplitude change with V . The change in shape leads to a halving of the persistent currents periodicity for high V .

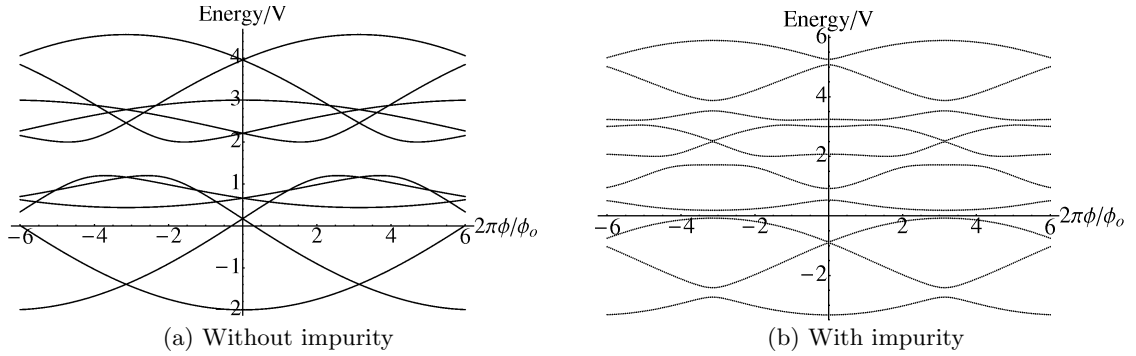


Figure 6.4: Comparison of the energy vs flux plots for a t - V ring with 5 sites and 3 particles with and without an impurity, with $t_N/t=2$ and $V/t=1$ and $\varepsilon=0$. It can be seen that the effect of the impurity is a lift of the energy degeneracy.

Conclusions

In this work we have addressed the topic of persistent currents in a ring enclosing a magnetic flux due to the Aharonov-Bohm effect. Periodic energy and magnetic moment in the magnetic flux was observed. The effects of the periodic lattice potential, disorder and Coulomb interaction were also addressed.

As we have shown, the results obtained for the persistent currents for the free electron gas model and for the tight-binding model converge very quickly with increasing number of sites. Convergence was expected in the thermodynamical limit but even so we have a strong convergence even for a small number of sites.

In the tight-binding model, the effect of having a single impurity treated using first order perturbation theory is rather trivial since the results obtained for the energy, magnetic moment and persistent currents are very similar to a tight-binding ring without impurities. Nevertheless, by using a numerical approach we have shown that the impurity can be responsible for a bound state, outside the usual range of the tight-binding band. We have also addressed a disordered ring using the tight-binding model and we have shown that averaging the persistent current over a large number of disordered configurations having the same Fermi energy results in a persistent current of the ensemble that has a superposition of characteristics from the persistent currents of single ring with an even number of electrons and of a single ring with an odd number of electrons.

We addressed the Coulomb interaction by studying a t-V ring and we have shown that some energy levels can have a decreased periodicity in the magnetic flux and amplitude when compared to the fundamental level. We have also shown that in the strong coupling limit the possible energy values are strongly localized around integer values of V . We have also concluded that the most evident effect of having an impurity in a t-V ring is the lift of the energy degeneracy as expected.

As future work, we would like to address different configurations with less symmetry than a ring. We would also like to study in detail the persistent currents in the t-V model using an analytical approach. Finally we would like to study the persistent currents for a more complex model, the extended Hubbard model, which makes use of the Hubbard and the t-V models.

Appendix A

Electromagnetic Hamiltonian

The classical electromagnetic Lagrangian will reproduce the Lorentz force if it's written as

$$L = \frac{1}{2}m\dot{\vec{r}} + q\dot{\vec{r}} \cdot \vec{A} - qV, \quad (\text{A.1})$$

where m is the particle's mass, $\dot{\vec{r}}$ is the particle's velocity, q is particle's charge, $\vec{A}$ is the particle's magnetic potential vector and V the electric potential.

The Hamiltonian of a system is given by

$$H = \vec{p} \cdot \dot{\vec{r}} - L, \quad (\text{A.2})$$

where $\vec{p}$ is the conjugate momentum. Therefore, the classical electromagnetic Hamiltonian can be written as

$$H = \frac{(\vec{p} - q\vec{A})^2}{2m} + qV. \quad (\text{A.3})$$

Appendix B

Second quantization Fermionic operators

Second quantization relies on the fermionic creation and annihilation operators. The creation operator, $c_{k,\sigma}^\dagger$, creates a fermion at site k with spin σ and his adjoint, the annihilation operator, $c_{k,\sigma}$, destroys a fermion at site k with spin σ . Because here we only work with spinless fermions we are going to drop the spin index, σ . The operations with creation and annihilation operators for spinless fermions follow the equations:

$$\begin{aligned}c_i^\dagger c_j + c_j c_i^\dagger &= \delta_{i,j} \\ c_i^\dagger c_j + c_j^\dagger c_i^\dagger &= 0 \\ c_i c_j + c_j c_i &= 0\end{aligned}\tag{B.1}$$

Though they are useful, in many situations it is easier to think in a more intuitive and less mathematical way. For example, imagine we operate a creation operator over a ring with N sites. Due to Pauli's exclusion principle, we cannot create a fermion at site 1 if there is already a fermion there. So, if we do so, the result will be the null vector: $c_1^\dagger |1\rangle = 0$. If we operate an annihilation operator over the vacuum, due to the fact that there aren't any fermions to destroy, the result will be the null vector too: $c_k |0\rangle = 0$.

Appendix C

Electrical current operator

C.1 Free electron gas

For the free electron case we have that the energy is given by

$$E = \frac{\hbar^2}{2m} k^2 \quad (\text{C.1})$$

where m is mass of the electron and

$$k = \frac{2\pi}{L} \left(n + \frac{\phi}{\phi_o} \right), \quad (\text{C.2})$$

where L is the ring radius, $n = 0, \pm 1, \pm 2, \dots$ is a quantum number and $\phi_o = h/e$ is the quantum of flux. Knowing that the electron's group velocity is given by $v_g = \frac{1}{\hbar} \frac{\partial E}{\partial k}$, we have

$$I = -\frac{ev_g}{L} = -\frac{e}{\hbar L} \frac{\partial E}{\partial k} = -\frac{e}{\hbar L} \frac{\partial E}{\partial \phi} \frac{\partial \phi}{\partial k}, \quad (\text{C.3})$$

and so we have

$$I = -\frac{\partial E}{\partial \phi} \quad (\text{C.4})$$

for the free electron case.

C.2 Tight-binding model

By definition,

$$\dot{n}_j = -\frac{i}{\hbar} [n_j, H]. \quad (\text{C.5})$$

Then by using the tight-binding Hamiltonian we have:

$$\dot{n}_j = \frac{it}{\hbar} \left(e^{i\phi'/N} c_j^\dagger c_{j+1} - e^{-i\phi'/N} c_{j+1}^\dagger c_j - e^{i\phi'/N} c_{j-1}^\dagger c_j + e^{-i\phi'/N} c_j^\dagger c_{j-1} \right). \quad (\text{C.6})$$

The continuity equation is given by

$$\dot{n}_j = j_{j-1} - j_j \quad (\text{C.7})$$

where j is the particle current operator per site. Eq. (C.7) is satisfied if

$$j_j = -\frac{it}{\hbar} \left(e^{i\phi'/N} c_j^\dagger c_{j+1} - e^{-i\phi'/N} c_{j+1}^\dagger c_j \right). \quad (\text{C.8})$$

Then we have for the total particle current,

$$\begin{aligned} J &= \frac{1}{N} \sum_{j=1}^N j_j \\ &= -\frac{it}{\hbar N} \sum_{j=0}^N \left[e^{i\phi'/N} c_j^\dagger c_{j+1} - e^{-i\phi'/N} c_{j+1}^\dagger c_j \right]. \end{aligned} \quad (\text{C.9})$$

For the electric current we have that $J_e = -eJ$ and so

$$J_e = -\frac{\partial H}{\partial \phi}. \quad (\text{C.10})$$

In a stationary case we can then write

$$I = -\frac{\partial E}{\partial \phi}. \quad (\text{C.11})$$

Appendix D

Wavefunctions for a free electron in a ring

For a free electron in a ring we have the following Schrödinger equation (forgetting about the magnetic vector potential for simplicity),

$$-\frac{\hbar^2}{2m}\nabla_{polar}^2\psi = E\psi, \quad (D.1)$$

where $\nabla_{polar}^2 = \frac{d^2}{d\theta^2}$ is the Laplacian operator in polar coordinates. We have then the following solution to equation (D.1),

$$\psi(\theta) = A.e^{i\sqrt{\frac{2mr^2E}{\hbar^2}}\theta}. \quad (D.2)$$

Because in a ring the electron's wavefunctions must be periodic and because of the normalization integral, we have the following two conditions,

$$\psi(\theta) = \psi(\theta + 2\pi), \quad (D.3)$$

$$\int_0^{2\pi} |\psi(\theta)|^2 d\theta = 1. \quad (D.4)$$

Applying the first condition.

$$e^{i\frac{r}{\hbar}\sqrt{2mE}\theta} = e^{i\frac{r}{\hbar}\sqrt{2mE}(\theta+2\pi)} \Leftrightarrow e^{i2\pi\frac{r}{\hbar}\sqrt{2mE}} = e^{i2\pi n} \Leftrightarrow E = \frac{n^2\hbar^2}{2mr^2}. \quad (D.5)$$

Applying the second condition.

$$\int_0^{2\pi} |A|^2 R d\theta = 1 \Rightarrow A = \frac{1}{\sqrt{2\pi R}}. \quad (D.6)$$

and so we have the electron's wavefunctions,

$$\psi_n(\theta) = \frac{1}{\sqrt{2\pi R}} e^{in\theta}. \quad (D.7)$$

Because in polar coordinates, a ring is merely a line with periodic boundary conditions, we can arrive at the same wavefunctions considering a linear one dimensional system with Born-von Karman boundary conditions.

Appendix E

Free electron persistent current calculation

The total current is given by

$$\begin{aligned}
 I_{Total}(\phi) &= \sum_{n'_F}^{n_F} I_n \\
 &= -\frac{\hbar e}{mL} \sum_{n'_F}^{n_F} (n) + \sum_{n'_F}^{n_F} \left(\frac{\phi}{\phi_o} \right),
 \end{aligned} \tag{E.1}$$

where $I_n = -\frac{\partial E_n}{\partial \phi}$.

Analyzing region $-0.5 < \phi/\phi_o < 0.5$ of Fig. E.1, we can easily see that the order of occupation will be different if we are in the region $-0.5 < \phi/\phi_o < 0$, where we will fill first $n = 0$ then $n = 1$, then $n = -1, \dots$, or in the region $0 < \phi/\phi_o < 0.5$, where we will fill first $n = 0$ then $n = -1$, then $n = 1, \dots$.

If the number of electrons is odd, the same levels will be filled if we are to the left of the energy axis or to the right. On the other hand if the number of electrons is even, the level

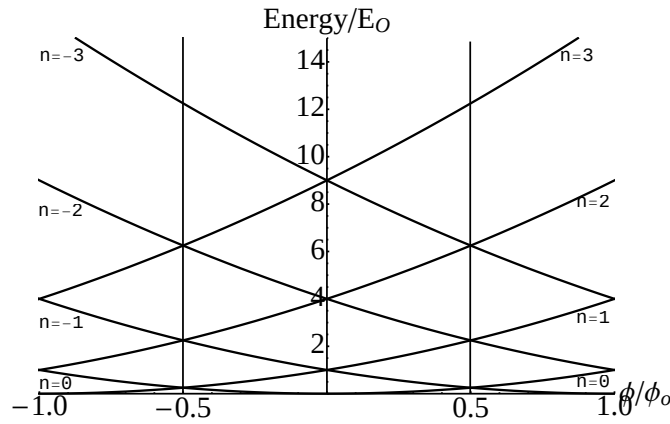


Figure E.1: Energy-flux graphic for the free electron gas.

filling will be different if we are to the left or to the right of the energy axis. To the left of the energy axis, because we will fill positive levels first, we will, if $N_e > 1$, always have $n_F = -n'_F + 1$ (remember that $n_F > 0$ and that $n'_F < 0$). To the right of the energy axis, if $N_e < 1$ we will have $n_F = -n'_F - 1$. Taking this in account we arrive at the expression for $I_{Total}(\phi)$:

$$I_{Total}(\phi) = \begin{cases} -I_o \frac{2\phi}{\phi_o}, & N_e \text{ odd}, \frac{\phi}{\phi_o} \in [-0.5, 0.5[\\ -I'_o \left(\frac{2\phi}{\phi_o} + 1 \right), & N_e \text{ even}, \frac{\phi}{\phi_o} \in [-0.5, 0[\\ -I'_o \left(\frac{2\phi}{\phi_o} - 1 \right), & N_e \text{ even}, \frac{\phi}{\phi_o} \in]0, 0.5[\end{cases} \quad (\text{E.2})$$

where

$$I_0 = \frac{\hbar e}{mL} \left(n + \frac{1}{2} \right), \quad (\text{E.3})$$

and

$$I'_0 = \frac{\hbar e}{mL} (n + 1). \quad (\text{E.4})$$

Appendix F

Tight-binding Hamiltonian in the presence of an external magnetic flux

Using nearest-neighbors approximation, the hopping factor is given by

$$\begin{aligned} t &= \int \phi^* (\vec{r}) h_1 \phi (\vec{r} - \vec{R}) d\vec{r} \\ &= \int \phi^* (\vec{r}) \left[\frac{1}{2m} (\vec{p} + e\vec{A})^2 \right] \phi (\vec{r} - \vec{R}) d\vec{r} \end{aligned} \quad (\text{F.1})$$

where ϕ are the Wannier functions, h_1 is the one-particle Hamiltonian and $\vec{R}$ is the lattice vector. Let's write the magnetic flux as $\lambda(\vec{x})$ (in order to avoid confusing it with the Wannier functions),

$$\lambda(\vec{r}) = \int_{\vec{r}_0}^{\vec{r}} \vec{A}(\vec{r}) d\vec{r} \quad (\text{F.2})$$

Eq. (F.1) can be written as

$$t_{ij} = \int \phi^* (\vec{r}) e^{-ie\lambda} \left[\frac{1}{2m} (\vec{p} + e\vec{A} - \vec{\nabla}\lambda(\vec{r}))^2 \right] e^{ie\lambda} \phi (\vec{r} - \vec{R}) d\vec{r}. \quad (\text{F.3})$$

By defining, $\tilde{\phi}(\vec{r} - \vec{R}) = e^{ie\lambda(\vec{r})} \phi(\vec{r} - \vec{R})$ the hopping matrix elements can be written as

$$t = \int \tilde{\phi}^* (\vec{r}) \left[\frac{\vec{p}^2}{2m} \right] \tilde{\phi} (\vec{r} - \vec{R}) d\vec{r}. \quad (\text{F.4})$$

Let us assume that the Wannier functions, $\phi(\vec{r} - \vec{R})$ are strongly localized around $\vec{R}$ and that $\vec{A}$ varies slowly on the atomic scale. Then we can say that

$$\tilde{\phi}(\vec{r} - \vec{R}) = e^{ie\lambda(\vec{R})} \phi(\vec{r} - \vec{R}), \quad (\text{F.5})$$

and we can write the tight-binding Hamiltonian as

$$H = -t \sum_{j=1}^N \left[e^{ie(\lambda(\vec{R}_{j+1}) - \lambda(\vec{R}_j))} c_j^\dagger c_{j+1} + h.c. \right], \quad (\text{F.6})$$

which, doing $\lambda \rightarrow \phi$ (since we don't need the Wannier functions anymore, we can use ϕ for the flux) is the same as,

$$H = -t \sum_{j=1}^N \left[e^{i\phi'/N} c_j^\dagger c_{j+1} + h.c. \right], \quad (\text{F.7})$$

where $\phi' = 2\pi \frac{\phi}{\phi_o}$, $\phi_o = \frac{e}{h}$.

Bibliography

- [1] H. F. Cheung, Y. Gefen, and E. Riedel. Isolated rings of mesoscopic dimensions, quantum coherence and persistent currents. *IBM J. Res. Develop.*, 32(3):359–371, May 1988.
- [2] H. F. Cheung, Y. Gefen, E. Riedel, and W. Shih. Persistent currents in small one-dimensional metal rings. *Phys. Rev. B*, 37(11):6050–6062, 15 April 1988-I.
- [3] E. M. Jariwala, P. Mohanty, M. b. Ketchen, and R. A. Webb. Diamagnetic persistent currents in diffusive normal-metal rings. *Phys. Rev. Lett.*, 86(8):1594–1597, 19 February 2001.
- [4] Y. Aharonov and D. Bohm. Significance of electromagnetic potentials in the quantum theory. *Phys. Rev.*, 115(3):485–491, 1 August 1959.
- [5] N. W. Ashcroft and N. D. Mermin. *Solid state physics*. Thomson Learning, 1976.
- [6] F. Reif. *Fundamental of statistical and thermal physics*. McGraw Hill Learning, 1984.
- [7] R. A. Webb, S. Washburn, C. P. Umbach, and R. B. Laibowitz. Observation of h/e aharonov-bohm oscillations in normal-metal rings. *Phys. Rev. Lett.*, 54(25):2696–2699, June 1985.
- [8] N. C. Koshnick, H. Bluhm, M. E. Huber, and K. A. Moler. Fluctuation superconductivity in mesoscopic aluminum rings. *Science*, 318(5855):1440–1443, 30 November 2007.
- [9] M. P. Marder. *Condensed Matter Physics*. Wiley-Interscience, 2000.
- [10] R. G. Dias. Exact solution of the strong coupling t-V model with twisted boundary conditions. *Phys. Rev. B*, 62(12):7791–7801, 15 September 2000-II.