UTRECHT UNIVERSITY
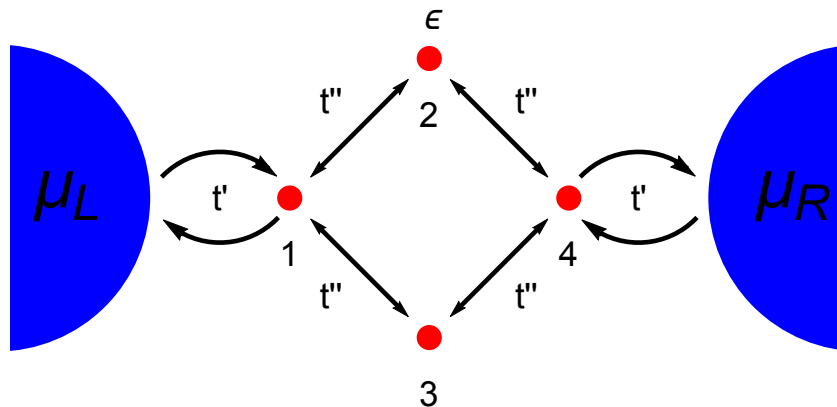
INSTITUTE OF THEORETICAL PHYSICS

Mesoscopic Electronic Transport through Ring-Shaped Nano-Structures

Author:

F.E.Elzinga,
3926850.

Supervisor:

Dr. D.Schuricht.

Co-supervisors:

N.Gergs, Msc.
B.Schönauer, Msc.

June 14, 2016

Abstract

In this thesis we investigate the mesoscopic electronic transport properties of ring-shaped nano-structures connected to two leads at low temperatures in the wideband limit. In particular we consider the current due to a constant chemical potential bias and the linear DC conductance. This is done in the Landauer-Büttiker formalism using equilibrium Green function techniques to compute transmission amplitudes.

The thesis starts with an introduction to second quantisation and derivations of the aforementioned formalism and techniques. We then move on to apply the theory to the specific cases of a single site impurity and an asymmetric four site ring.

We find that the transmission amplitude as a function of energy is sharply peaked around energy levels of the nano-structure, but has finite width and a small shift in resonance due to effective broadening by the coupling between leads and nano-structure. In the four site ring we also find signs of self-interference effects when the energy of the incoming electron is exactly half of the on-site energy.

We conclude with a discussion of possible generalisations of our model and a schematic overview of the necessary techniques, and areas of current research.
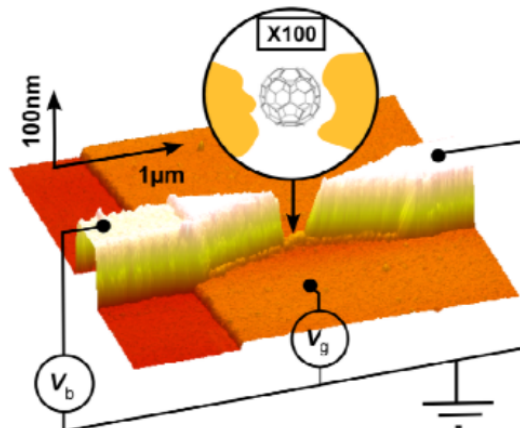
Contents

Contents

1 Introduction

Figure 1.1: An Atomic Force Microscopy image of a C_{60} molecule trapped between two gold nano-wires, to illustrate an appearance of the type of systems we are discussing (taken from [15]).

One of mankind's most impactful inventions of the past century was probably the computer. It brought with it the onset of the current information age, wherein any person at any given time is highly likely to be using or at least carrying with them a computer-like device (such as a smartphone, a laptop, etc.). The first computers were large machines that took up entire rooms, and were less powerful than the phone the author usually carries in his pocket. This miniaturisation was made possible by the invention of transistors, inherently quantum-mechanical devices that operate on the nanometre scale.

However, the theoretical and practical limitations of this technology are in sight and new methods are needed. This has sparked interest for fundamental research into the electronic transport properties of small systems (which we will often refer to as nano-structures). At low temperatures, the microscopic properties of such systems start to dominate the transport qualities as Ohmic behaviour breaks down. This is due to the fact that in these systems the electron mean free path length (and other coherence lengths) are not small compared to the system size (in fact they may even be much larger). Hence statistical, bulk descriptions fail, and microscopic details need to be taken into account (see the introductions to [6] and [9]). This blend between macro- and microscopic physics has lead these system to be dubbed *mesoscopic*. For example, conductance is no longer a bulk property, but rather is related to the geometry of the system via transmission functions.

The experimental realisability of these systems has made direct comparison between theory and experiment possible (see [19] and [3]), resulting in active theoretical research driven by experiment. Popular systems to study include molecules (see fig.1.1), quantum dots, and point contacts on semiconductors.

A simple yet powerful theoretical approach to the transport properties these system comes in the form of the *Landauer-Büttiker formalism*, which will be discussed in chapter 4, after the stage has been set with the necessary background information in chapters 2 and 3. In chapter 5 we present a Green function approach that will take care of the microscopic details. Chapters 6 and 7 will then be dedicated to

specific model systems, and finally, in chapter 8 we discuss how these models may be extended and provide a sketch of the necessary methods.

2 Second Quantisation

An invaluable set of tools that we will need to do microscopic calculations is provided by the formalism of *second quantisation*. It provides an elegant and powerful quantum mechanical approach to many body physics. The name is unfortunately a historical misnomer, in the sense that one does not quantise *again* in this approach, but rather one switches to a fully quantum mechanical perspective and most of all notation. The method was introduced by Paul Dirac[1] in the late twenties and further developed later by many others, with notable contributions by Vladimir Fock[2] and Pascual Jordan[3]. The building blocks of the theory are the first quantisation approach to single-particle quantum mechanics (taught in all elementary courses) and two additional postulates, namely that the particles the theory treats are fundamentally indistinguishable and that few-particle operators retain their first quantised form. Over the course of the next few sections a schematic derivation of the theory for spinless fermions will be given. For a more complete treatment we refer to [4].

2.1 First Quantisation

In this section we will review some basics of first quantisation to set the stage for second quantisation and to recall some results that will be useful later. For details one could consult [8], or for a more formal reference [17]. Recall from elementary quantum mechanics that (in the Schrödinger picture) a single particle system is described by a wave function $\Psi : \mathbb{R}^3 \times \mathbb{R} \to \mathbb{C}$, that lives in a Hilbert space $\mathcal{H}$, whose evolution in time is governed by the *Schrödinger equation*[4]

$$i\hbar \partial_t \Psi = H\Psi = \left(-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}} + V(\mathbf{r}) \right) \Psi. \tag{2.1.1}$$

One should view $\mathcal{H}$ as a "nice" space containing "physically relevant" wave functions, i.e. these go (sufficiently quickly) to zero at infinity, are as smooth as they need to be for our manipulations, et cetera. According to Max Born's[5] statistical interpretation of the wave function, one should view

$$\int_U d\mathbf{r} \ |\Psi(\mathbf{r}, t)|^2 \tag{2.1.2}$$

as the probability to find the particle in the region of space U at time t. This immediately imposes the condition that any wave function must be normalised such that we have

$$\int_{\mathbb{R}^3} d\mathbf{r} \ |\Psi(\mathbf{r}, t)|^2 = 1.$$

Thus the wave function is also required to be square integrable over the whole space, for all times. One may wonder if it is possible to achieve this normalisation, since

---

[1] 1902-1984, English, awarded the 1933 Nobel Prize together with Erwin Schrödinger (will be mentioned again later) for their work on atomic physics.

[2] 1898-1974, Russian.

[3] 1902-1980, Prussian/German, not to be confused with the French mathematician Camille Jordan.

[4] named after Erwin Schrödinger, 1887-1961, Austrian, see the footnote on Paul Dirac.

[5] 1882-1970, German, he was awarded the 1954 Nobel prize for this insight.

the wave function may also vary in time. As it turns out, a wave function that is normalised at one point in time, will be normalised for all points in time. We will prove this here as the proof contains a result that will be used to derive the Landauer-Büttiker formula (see chapter 4, a more general form will also be used in chapter 8). Since differentiation with respect to time and integration over space commute, it suffices to consider

$$\partial_t|\Psi|^2 = \Psi^*\partial_t\Psi + \Psi\partial_t\Psi^* = \Psi^*\left(\frac{i\hbar}{2m}\Delta\Psi - \frac{i}{\hbar}V\Psi\right) + \left(-\frac{i\hbar}{2m}\Delta\Psi^* + \frac{i}{\hbar}V\Psi^*\right)\Psi,$$

$$= \nabla\cdot\left[\frac{i\hbar}{2m}\left(\Psi^*(\nabla\Psi) - \text{c.c}\right)\right] =: -\nabla\cdot\mathbf{J}, \tag{2.1.3}$$

where we have used (2.1.1) and its complex conjugate, and $\mathbf{J}$ is the so called *probability current density*. We can now directly compute

$$\mathrm{d}_t\int_{\mathbb{R}^3}\mathrm{d}\mathbf{r}\ |\Psi|^2 = \int_{\mathbb{R}^3}\mathrm{d}\mathbf{r}\ \partial_t|\Psi|^2 = -\int_{\mathbb{R}^3}\mathrm{d}\mathbf{r}\ (\nabla\cdot\mathbf{J}) = -\lim_{\rho\to\infty}\int_{S_\rho^2}\mathbf{J}\cdot\mathrm{d}\mathbf{S} = 0.$$

The last two steps follow from the Gauß-Ostrogradsky theorem[6], the definition of the improper Riemann integral, and from the fact that the wave function and its derivatives go to zero at infinity and hence so does $\mathbf{J}$.

In the case of a time independent problem, the situation simplifies considerably. One then uses the (perhaps even more famous) *time independent Schrödinger equation*

$$H\psi = E\psi, \tag{2.1.4}$$

which one can derive by separation of variables. This is an eigenvalue problem and since energy must be real, H must be an Hermitian operator. It then follows from the spectral theorem for self-adjoint operators (the mathematician's word for Hermitian) that there exists a complete orthonormal basis of eigenvectors (called *eigenstates* in physics) indexed by some multi-index of quantum numbers ν. These indices may be discrete, continuous or consist of both types. Hence (2.1.4) always has solutions, a comparable statement can be proven for the full equation (2.1.1). Such a set is usually denoted as $\{\psi_\nu\}$ and the above properties can be stated as the following identities that are fundamental to quantum mechanics

$$\sum_\nu \psi_\nu^*(\mathbf{r}')\psi_\nu(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}') \qquad \text{(completeness)}, \tag{2.1.5}$$

$$\int\mathrm{d}\mathbf{r}\ \psi_{\nu'}^*(\mathbf{r})\psi_\nu(\mathbf{r}) = \delta_{\nu\nu'} \qquad \text{(orthonormality)}. \tag{2.1.6}$$

One should be mindful of the notation used here, the sum over ν is to be interpreted as an integral if the quantum number is continuous, and as an appropriate product of sums and integrals if ν contains several quantum numbers. The upper delta is the so called *Dirac delta*[7], and the lower one the *Kronecker delta*, both will make numerous appearances in what is to come. From now on we will work with these time independent wave functions.

---

[6]This theorem has been independently discovered by several famous mathematicians, but most prominently by Johann Karl Friedrich Gauß(1777-1855, German), it was however first proven by Mikhail Ostrogradksy (1801-1862, Russian).

[7]Popularised by Paul Dirac in his 1930 book *"The Principles of Quantum Mechanics"*

2.2   Many Particle Wave Functions

The goal is now to somehow extend this approach to systems of several particles, say N. What is meant in this case by the *many particle wave function* Ψ (or more specifically the N-particle wave function) is again an element of some Hilbert space $\mathcal{H}'$. However this time the domain is not real space but rather the $3N$ dimensional *configuration space* of the system, which we may identify with $\mathbb{R}^{3N}$. In this context we interpret

$$\int_U \mathrm{d}\mathbf{r}_1 \cdots \mathbf{r}_N |\Psi(\{\mathbf{r}_i\})|^2$$

as the probability to find the system in the region U of the configuration space, in the spirit of (2.1.2). If we assume that $\mathcal{H}'$ contains all N-particle wave functions for some system, for all N, then we have $\{\psi_\nu\} \subset \mathcal{H}'$ (we will propose a concrete candidate for this space later). We will now show that any Ψ can be constructed out of these states. We define the function $C(\nu_1, \{\mathbf{r}_i\}_{N \geq i \geq 2})$ by projecting onto the single particle state ν_1 as follows

$$C_1 = C(\nu_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) := \int \mathrm{d}\mathbf{r}_1 \ \psi_{\nu_1}^*(\mathbf{r}_1)\Psi(\{\mathbf{r}_i\}),$$

and iteratively the other $N-1$ functions

$$C_j = C(\nu_1, \ldots, \nu_j, \mathbf{r}_{j+1}, \ldots, \mathbf{r}_N) := \int \mathrm{d}\mathbf{r}_j \ \psi_{\nu_j}^*(\mathbf{r}_j) \ C_{j-1}.$$

Note that the N-th iteration simply gives us a collection of complex numbers indexed by $\{\nu_i\}$. We can use (2.1.5) to invert any one of these steps by computing

$$\sum_{\nu_j} \psi_{\nu_j}(\mathbf{r}_j')C_j = \int \mathrm{d}\mathbf{r}_j \left[\sum_{\nu_j} \psi_{\nu_j}(\mathbf{r}_j')\psi_{\nu_j}^*(\mathbf{r}_j) \right] C_{j-1} = \int \mathrm{d}\mathbf{r}_j \delta(\mathbf{r}_j - \mathbf{r}_j')C_{j-1},$$

$$= C(\nu_1, \ldots, \nu_{j-1}, \mathbf{r}_j', \ldots, \mathbf{r}_N).$$

It is easy to check that this procedure maps C_1 back to Ψ and hence we find that

$$\Psi(\{\mathbf{r}_i\}) = \sum_{\{\nu_i\}} C_N(\{\nu_i\})\psi_{\nu_1}(\mathbf{r_1}) \cdots \psi_{\nu_N}(\mathbf{r}_N). \tag{2.2.1}$$

In other words, we have shown that the collection

$$\left\{ \prod_{i=1}^N \psi_{\nu_i}(\mathbf{r}_i) \ : \ \forall N \in \mathbb{N}, \ \forall\{\nu_i\} \right\}$$

is a basis of $\mathcal{H}'$.

To find out more information about the coefficients, we explore the consequences of the indistinguishable particles postulate. If we define the permutation operator P_{ij} that interchanges particles i and j, this operator acting on some state should yield the same physical answers as an unaffected state (as the particles are indistinguishable). This implies that P_{ij} can be at most multiplying the permuted state by some complex number p, and moreover that applying the operator twice should lead to exactly the

same state, i.e. $p^2 = 1$. It follows that $p = \pm 1$ and by the spin statistics theorem that $p = -1$ corresponds to fermions and $p = 1$ to bosons. It should be noted that this argument only holds in three (or more) spatial dimensions, since in lower dimensions the square of the permutation operator is not necessarily homotopy equivalent to the identity (loosely speaking one cannot exchange two particles without disturbing the particles in between). There is experimental evidence for the existence of quasi-particles that do in fact exhibit different phases under adiabatic exchange, for example the fractional quantum hall effect. In the case of fermions, $p = -1$ means that the coordinates $\{\mathbf{r}_i\}$ should appear in a completely antisymmetric way. A common way of achieving this in physics is to use the so called *Slater determinant*

$$\mathcal{A}\left(\prod_{i=1}^{N} \psi_{\nu_i}(\mathbf{r}_i)\right) = \sum_{\sigma \in \mathcal{S}_n} \text{sign}(\sigma) \prod_{i=1}^{N} \psi_{\nu_{\sigma(i)}}(\mathbf{r}_{\sigma(i)}). \tag{2.2.2}$$

Notice that if one were to apply this operator to a product of single particle states where not all quantum numbers are distinct, the result would be zero. This is known as the *Pauli exclusion principle*, in other words, no two fermions may occupy the same quantum state. These symmetry requirements are hidden in the coefficients $C_N(\{\nu_i\})$ and additionally it means that states such as $\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2)$ are not physical. So in a sense this hypothetical Hilbert space $\mathcal{H}'$ contains much more then is needed. In the over-next section we will discuss a trimmed down Hilbert space together with some very slick notation that will be much more convenient.

2.3 A Brief Mathematical Digression

From our computation in the previous section it is clear that the space $\mathcal{H}'$ corresponds to

$$\mathcal{H}' = \overline{\bigoplus_{i=0}^{\infty} \mathcal{H}_i},$$

where $\mathcal{H}_i$ denotes the i-particle Hilbert space

$$\mathcal{H}_i := \begin{cases} \displaystyle\bigotimes_{j=1}^{i} \mathcal{H} & i \geq 1 \\ \text{span}\{|0\rangle\} \cong \mathbb{C} & i = 0 \end{cases},$$

the bar indicates that we take the completion[8], and $|0\rangle$ denotes the *vacuum state* (not to be confused with the ground state), i.e. a completely empty system (we will use Dirac notation from now on). This space is usually called *Fock space* and denoted as $\mathcal{F} := \mathcal{H}'$. By the Fréchet-Riesz representation theorem we may identify these tensors with our wave functions. Our discussion indicates that the physically relevant subspace for fermions is in fact the exterior algebra of $\mathcal{H}$, in symbols $\mathcal{F}_f := \overline{\Lambda^* \mathcal{H}}$. Since this space is also the result of a direct sum, it has the property that states with different amounts of particles are orthogonal. We recall that the multiplication on

---

[8]This not only ensures that the space remains Hilbert, but additionally there are physically relevant states that we would discard otherwise, such as the so called *coherent states* $|\phi\rangle = \exp(\phi a^\dagger)|0\rangle$, which are eigenstates of the annihilation operator (defined in the next section).

the exterior algebra is given by the wedge product $\wedge$ (sometimes also called exterior product)[9], which allows us to write a basis of fermionic Fock space as

$$\left\{ \bigwedge_{i=1}^{N} |\psi_{\nu_i}\rangle \ : \ \forall N \in \mathbb{N}, \ \forall \{\nu_i\} \right\}. \tag{2.3.1}$$

Note that not only the antisymmetry requirement, but also the Pauli principle is build into these states, since $a \wedge a = 0$ for any $a \in \overline{\Lambda^* \mathcal{F}}$. Moreover the order of $\{\nu_i\}$ is important since $a \wedge b = -b \wedge a$, which one can view as a residual artefact of trying to label or order the particles. In the next section we will take a more physical approach to remedy these last hiccups. We will not use any of the algebraic properties directly, but they will be hidden inside the definitions of operators and their (anti)commutation relations.

2.4 The Occupation Number Representation

The treatment up to this point should convince us that we must forgo any attempt to build a many particle wave function out of the particles it describes. Rather it has become clear that the physical content of such a wave function is not "which particle is in what state", but "how many particles are in each state". At this point we should fix an ordering of the single particle quantum states. This ordering is of course arbitrary, but must be used consistently. We now introduce that objects $\{|\{n_{\nu_i}\}\rangle\}$, where n_{ν_i} is the *occupation number* of the state ν_i. Concretely we have reduced the size of (2.3.1) without losing its spanning property by imposing a fixed order and have defined the N-particle wave functions

$$\left| n_{\nu_{i_1}}, \ldots, n_{\nu_{i_N}} \right\rangle := \left| \psi_{\nu_{i_1}} \right\rangle \wedge \cdots \wedge \left| \psi_{\nu_{i_N}} \right\rangle =: |\nu_{i_1}\rangle \wedge \cdots \wedge |\nu_{i_N}\rangle.$$

We will often write $n_{\nu_{i_j}} = n_{i_j}$, which is unambiguous because we have imposed an order on the quantum labels. This is called the *occupation number representation* and it constitutes a lean, elegant, and efficient way to write down many particle wave functions.

The most natural operator to define now is the operator that when unleashed returns the occupation number of a certain state, in symbols

$$\hat{n}_i |\{n_j\}\rangle := n_i |\{n_j\}\rangle,$$

which defines it on the entire space $\mathcal{F}_f$. Two more natural operators that will turn out to be intimately linked to the particle number operator are the *creation* and *annihilation* operators $a_{\nu_j}^{\dagger}$ and a_{ν_j}. We begin by defining the former by demanding

$$a_{\nu_j}^{\dagger} |n_{i_1}, \ldots, n_{i_j}, \ldots, n_{i_N}\rangle = C(n_{i_j}) |n_{i_1}, \ldots, n_{i_j} + 1, \ldots, n_{i_N}\rangle.$$

Since we have

$$\left| n_{i_1}, \ldots, n_{i_j}, \ldots, n_{i_k}, \ldots, n_{i_N} \right\rangle = -\left| n_{i_1}, \ldots, n_{i_k}, \ldots, n_{i_j}, \ldots, n_{i_N} \right\rangle, \tag{2.4.1}$$

---

[9]Usually $a \wedge b := a \otimes b \pmod{I}$, where I is the two-sided ideal generated by elements of the form $c \otimes c$, i.e. $c \wedge c = 0$ for all c. This also immediately implies that the wedge product is alternating, since $0 = (a+b) \wedge (a+b) = a \wedge b + b \wedge a$.

it must also hold that $\{a^\dagger_{\nu_j}, a^\dagger_{\nu_k}\} = 0$, where we have introduce the *anticommutator* $\{a, b\} := ab + ba =: [a, b]_+$. The relation between $a^\dagger_{\nu_j}$ and a_{ν_j} follows from (we only write the relevant occupation number)

$$\langle n_{\nu_j} + 1 | a^\dagger_{\nu_j} | n_{\nu_j} \rangle^* = \langle n_{\nu_j} | (a^\dagger_{\nu_j})^\dagger | n_{\nu_j} + 1 \rangle = \langle n_{\nu_j} | a_{\nu_j} | n_{\nu_j} + 1 \rangle, \qquad (2.4.2)$$

so a_{ν_j} is indeed an annihilation operator that sends

$$a_{\nu_j} | n_{\nu_j} \rangle = A(n_{\nu_j}) | n_{\nu_j} - 1 \rangle.$$

By taking adjoints a_{ν_j} and a_{ν_k} must also satisfy $\{a_{\nu_j}, a_{\nu_k}\} = 0$, thus $(a^\dagger_{\nu_j})^2 = (a_{\nu_j})^2 = 0$. Applying the same arguments based on (2.4.1) as above it must also hold that $\{a_{\nu_j}, a^\dagger_{\nu_k}\} = 0$ for $j \neq k$. We also demand that

$$a_{\nu_j} | 0 \rangle = 0, \ a^\dagger_{\nu_j} | 0 \rangle = | 0, \ldots, 0, n_{\nu_j} = 1, 0, \ldots \rangle,$$

the second condition simply being a normalisation. Hence $C(0) = 1$, $A(0) = 0$, and $A(1) = 1$ (use (2.4.2)) and we can compute

$$\{a_{\nu_j}, a^\dagger_{\nu_j}\} | 0 \rangle = | 0 \rangle.$$

We now assume that we can extend this to the operator identity $\{a_{\nu_j}, a^\dagger_{\nu_j}\} = 1$. This gives us the full algebra of the creation and annihilation operators, namely the anticommutation relations

$$\{a_{\nu_j}, a_{\nu_k}\} = 0, \ \{a^\dagger_{\nu_j}, a^\dagger_{\nu_k}\} = 0, \ \{a_{\nu_j}, a^\dagger_{\nu_k}\} = \delta_{\nu_j \nu_k}. \qquad (2.4.3)$$

At this point we introduce a useful identity whose proof is nothing more than expanding definitions. Let A, B, and C be operators, denote their commutator by $[A, B]_- := [A, B]$ and let $\sigma = \pm 1$, then[10]

$$[A, BC]_\sigma = [A, B]_{\pm\sigma} C \mp \sigma B [A, C]_\pm. \qquad (2.4.4)$$

We now turn our attention to the operator $a^\dagger_\nu a_\nu$, for which it is easy to see that $| n_\nu = 0 \rangle$ and $| n_\nu = 1 \rangle$ are eigenstates with eigenvalues 0 and 1 respectively, which are exactly the occupation numbers. Using the commutators

$$[a^\dagger_\nu a_\nu, a_\nu] = -a_\nu, \ [a^\dagger_\nu a_\nu, a^\dagger_\nu] = a^\dagger_\nu, \qquad (2.4.5)$$

which one can derive from (2.4.4), we find that $(a^\dagger_\nu a_\nu)^2 = a^\dagger_\nu a_\nu$, hence the only possible eigenvalues are 0 and 1, as we expected. So indeed we have that $\hat{n}_\nu = a^\dagger_\nu a_\nu$.

2.5 Operators in Second Quantisation

To complete our discussion of second quantisation we need a few facts about the representation of general single site/particle operators. The key component is the observation that

$$\mathcal{A}\left(\prod_{j=1}^N \psi_{\nu_{i_j}}(\mathbf{r}_j)\right) = | n_{\nu_{i_1}} = 1, \ldots, n_{\nu_{i_N}} = 1 \rangle = a^\dagger_{\nu_{i_1}} \cdots a^\dagger_{\nu_{i_N}} | 0 \rangle.$$

---

[10]The way this equation is read is to pick σ on the left and then read either all upper or all lower sign on the right side.

One of our postulates was that few-particle operators do not change, by which we mean that if one wants to determine say p_i, the momentum of the particle in state i, from a many-particle wavefunction, one can simply apply the operator $\mathrm{id} \otimes \cdots \otimes \hat{p} \otimes \mathrm{id} \otimes \cdots$, where $\hat{p}$ is in position i[11]. In other words we postulate that to determine a property[12] of a single particle, we can forget about all other particles present in the system. This immediately implies that any operator acting on the system on a particle by particle basis can be simply regarded as the sum of these individual operators, in symbols

$$\hat{O}_{\text{tot}} = \sum_{i=1}^{N} \hat{O}_i.$$

Combining now our observation with the identity from elementary quantum mechanics

$$\hat{O}_i = \sum_{\nu_a \nu_b} O_{\nu_b \nu_a} \left| \nu_b \right\rangle \left\langle \nu_a \right| := \sum_{\nu_a \nu_b} \left(\left\langle \nu_b \right| \hat{O}_i \left| \nu_a \right\rangle \right) \left| \nu_b \right\rangle \left\langle \nu_a \right|,$$

and exploiting the properties of the creation and annihilation operators yields the general formula

$$\hat{O} = \sum_{\nu_a \nu_b} O_{\nu_b \nu_a} a_{\nu_b}^\dagger a_{\nu_a}. \tag{2.5.1}$$

One could interpret this identity to mean that an operator removes a particle from state ν_a and adds one to the state ν_b with weight $O_{\nu_b \nu_a}$. This also tells us what the creation and annihilation operators do to general states

$$a_{\nu_j} \left| \{ n_{\nu_i} \} \right\rangle = (-1)^{\sum_{l=1}^{j-1} n_{\nu_l}} n_{\nu_j} \left| n_{\nu_1}, \ldots, 1 - n_{\nu_j}, \ldots \right\rangle,$$
$$a_{\nu_j}^\dagger \left| \{ n_{\nu_i} \} \right\rangle = (-1)^{\sum_{l=1}^{j-1} n_{\nu_l}} (1 - n_{\nu_j}) \left| n_{\nu_1}, \ldots, 1 - n_{\nu_j}, \ldots \right\rangle,$$

which once again reinforces how important the ordering of the states is.

The final thing to consider are changes of basis, which we only need to do for the creation and annihilation operators by (2.5.1). The situation is no different from first quantisation, in that

$$\tilde{a}_\mu = \sum_\nu \left\langle \tilde{\psi}_\mu \middle| \psi_\nu \right\rangle a_\nu, \ \tilde{a}_\mu^\dagger = \sum_\nu \left\langle \tilde{\psi}_\mu \middle| \psi_\nu \right\rangle^* a_\nu^\dagger.$$

These transformations have two very important properties that validate them, namely they preserve the algebra of the creation and annihilation operators (transformations with this property are called *canonical*) and the total number of particles. The first statement is immediate from the linearity of the transformations and the anticommutator. The second statement follows from the computation

$$\sum_\mu \tilde{a}_\mu^\dagger \tilde{a}_\mu = \sum_\mu \sum_{\nu_1 \nu_2} \left\langle \psi_{\nu_1} \middle| \tilde{\psi}_\mu \right\rangle \left\langle \tilde{\psi}_\mu \middle| \psi_{\nu_2} \right\rangle a_{\nu_1}^\dagger a_{\nu_2} = \sum_{\nu_1 \nu_2} \left\langle \psi_{\nu_1} \middle| \psi_{\nu_2} \right\rangle a_{\nu_1}^\dagger a_{\nu_2}$$
$$= \sum_{\nu_1} a_{\nu_1}^\dagger a_{\nu_1}.$$

---

[11]One might argue that this is part of the postulate that established the existence of the many-particle wavefunction, but for clarity we present them as separate here.

[12]That is, a property from single-particle quantum mechanics.

3   Assumptions and Specifics of the Model

Now that we have the necessary vocabulary for many-body quantum mechanics, it is time to discuss the family of models we will be using throughout this thesis.

We consider a ring-shaped nano-structure that is connected to several (usually two in this thesis) reservoirs of electrons via identical leads[13] (see fig.3.2). Our first assumption is that all of these reservoirs are macroscopic, in thermal equilibrium, and isolated from each other. This means that we may use equilibrium statistical physics for the reservoirs when deriving an expression for the current in the system, even though we are treating a transport problem[14]. Specifically, we will use Fermi-Dirac statistics to determine the availability of electrons in certain states. Since our reservoirs are macroscopic, electrons leaving or entering will have negligible effects on for example the chemical potential of the reservoir. As we are not interested in reflections off of the reservoirs, we assume that the leads connecting the reservoirs to the dot (from quantum dot, used interchangeably here with nano-structure) are infinitely long (i.e., connection to the dot at $n = 0$, the reservoir at $n \to \infty$). Also we use the simplest model possible to describe these leads, as we are not interested in their properties.

This model will be a tight-binding approach[15], where we assume that our Warnier states are so strongly localised that we may take them to be delta functions at each site, yet the hopping amplitude t remains finite and is the same in all leads (See fig.3.1). Additionally we work at low temperatures so that we may neglect phonons. All of the above is captured in the Hamiltonian

$$H_{\text{res}} = H_r = \sum_{\alpha} H_r^{\alpha} = -t \sum_{\alpha,n} \left[c_{\alpha,n}^{\dagger} c_{\alpha,n+1} + \text{h.c.} \right]. \tag{3.0.1}$$

It will often turn out to be more convenient to work in momentum space where (3.0.1) is diagonal,

$$
\begin{aligned}
H_r^{\alpha} &= -\frac{t}{N} \sum_n \left[\left(\sum_k e^{-ikn} c_k^{\dagger} \right) \left(\sum_{k'} e^{ik'(n+1)} c_{k'} \right) + \text{h.c.} \right], \\
&= -\frac{t}{N} \left[\sum_{k,k'} e^{ik'} \left(\sum_n e^{-in(k-k')} \right) c_k^{\dagger} c_{k'} + \text{h.c.} \right], \\
&= -t \sum_k \left[e^{ik} c_k^{\dagger} c_k + \text{h.c.} \right], \\
&= \sum_k [-2t \cos(k)] c_k^{\dagger} c_k = \sum_k \epsilon_k \hat{n}_k.
\end{aligned}
\tag{3.0.2}
$$

In this approach we only look at one band and we also completely neglect any cross-sectional structure that the wave functions may posses. Since the dot has no such structure, it cannot have an effect on our answer and only serves to create more

---

[13]Identical in the sense that they have the same hopping parameter t and coupling strength t', see below.

[14]However this is still a full non-equilibrium problem.

[15]Another reason for this approach is that there are numerical results available for these types of systems, and simulations are inherently discrete.
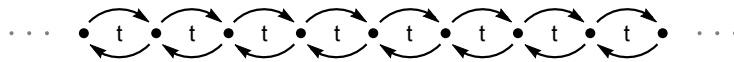
Figure 3.1: A cartoon of the tight binding model of the leads described in this section.

transport modes in the wire, which could be incorporated via some pre-factor if needed.

This ties in with our assumption that the charge carriers (we will use this word and "electrons" interchangeably) in the leads and the dot are spinless fermions, so we do not have to worry about any spin effects (again our dot has no spin or spin-coupling to speak of, so it is irrelevant). In general we assume our charge carriers to be non-interacting, and the transport to be coherent, i.e. the charge carriers always stay at the same momentum (elastic scattering). When we calculate the current later on we will consider a constant symmetric chemical potential bias of some width V which is centred about the middle of this cosine band.

The dot consists of several sites arranged in a ring-like structure between which electrons may hop and we associate to each site an energy. In symbols

$$H_{\mathrm{dot}} = H_d = \sum_\gamma \epsilon_\gamma d_\gamma^\dagger d_\gamma - \sum_{\gamma,\gamma'} t_{\gamma,\gamma'} d_\gamma^\dagger d_{\gamma'}, \tag{3.0.3}$$

where it should be noted that $t_{\gamma,\gamma'} = t_{\gamma',\gamma}$. Recall from our discussion of second quantisation that we should fix an ordering of the sites when we start to work with a concrete system. This will be done when we do so.

We now need a *tunnelling Hamiltonian* (we will sometimes also call it the tunnelling operator) that connects the leads to the dot. This is clearly achieved by

$$H_{\mathrm{tunnel}} = H_t = \sum_\beta H_t^\beta = -\sum_\beta t_\beta \left[c_{\beta,1}^\dagger d_{\beta,0} + \mathrm{h.c.} \right], \tag{3.0.4}$$

where $(\beta, 0)$ denotes the site in the dot where the lead is connected, so this site is part of the dot, not the lead.

Thus our total Hamiltonian will be

$$H = \sum_{\alpha,k} \epsilon_k c_{\alpha,k}^\dagger c_{\alpha,k} - \sum_\beta t_\beta \left[c_{\beta,1}^\dagger d_{\beta,0} + \mathrm{h.c.} \right] + \sum_\gamma \epsilon_\gamma d_\gamma^\dagger d_\gamma - \sum_{\gamma,\gamma'} t_{\gamma,\gamma'} d_\gamma^\dagger d_{\gamma'},$$

which acts on a Hilbert space that has the structure

$$\mathcal{H} = \mathcal{H}_{\mathrm{res}} \oplus \mathcal{H}_{\mathrm{dot}} \oplus \mathcal{H}_{\mathrm{res}},$$

where the reservoir spaces are infinite dimensional, but the dot space is finite dimensional. In particular it is no loss to view $H_{\mathrm{r/d}} : \mathcal{H}_{r/d} \to \mathcal{H}_{r/d}$, but this does not apply to $H_{\mathrm{t}} : \mathcal{H} \to \mathcal{H}$. These observations will be reflected in the computations in later sections, and in particular we shall see that the latter one can become very problematic (see chapter 8). One could say that H_t causes a hybridisation of the different parts of the Hilbert space, and if this is only a weak coupling, one expects the physics to be for the most part interpretable in terms of processes within the subspaces. This will indeed turn out to be the case if we consider a certain physical limit (the *wideband limit*).
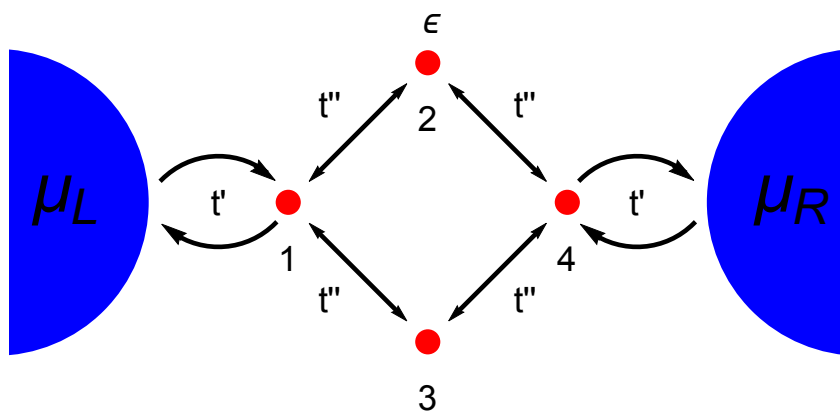
Figure 3.2: A cartoon of the model for the case of a 4 site ring with two identical connecting leads and uniform hopping within the dot and an on-site energy ϵ at the upper link.

4 The Landauer-Büttiker Formalism

As an Ansatz for the wave function caused by an electron coming from reservoir α with momentum k, we recall from the previous section that in the reservoirs, the electrons are free, hence their wave functions are plane waves. In a sense we zoom out so that we only see the reservoirs, which is meaningful since experimentally one measures the current across the entire system. Additionally the way we "measure" here is using so called *quantum point contacts*, i.e. we do not consider the effect of the structure of the measuring device on the system[16]. So it is natural to write

$$\langle n, \beta | \psi_{\alpha,k} \rangle = \frac{1}{\sqrt{2\pi}} \begin{cases} e^{-ikn} + R_\alpha(E_k)e^{ikn} & \alpha = \beta \\ T_{\beta,\alpha}(E_k)e^{ikn} & \alpha \neq \beta \end{cases}. \tag{4.0.1}$$

The quantities that we are interested in are the *reflection coefficient* $R_\alpha(E_k)$ and the *transmission coefficient* $T_{\beta,\alpha}(E_k)$. Since we use only positive k, the relation between E_k and k is one to one, and hence letting the coefficients be functions of E_k is unambiguous. Naturally we demand that probability is conserved, i.e.

$$|R_\alpha(E_k)|^2 + \sum_{\beta \neq \alpha} |T_{\beta,\alpha}(E_k)|^2 = 1, \tag{4.0.2}$$

of which we will show that it holds in general later. The normalisation follows from the condition $\langle \psi_{\alpha,k} | \psi_{\alpha,k'} \rangle = \delta(k - k')$, this is straightforward to check (keeping in mind that parts of the wave function in different leads are orthogonal). Another identity that is the linchpin of this normalisation calculation is

$$\sum_{\beta \neq \alpha} |T_{\beta,\alpha}(E_k)|^2 = \sum_{\beta \neq \alpha} |T_{\alpha,\beta}(E_k)|^2, \tag{4.0.3}$$

which we will also derive later once we have explicit formulae for the coefficients.

We now use our assumption of macroscopic reservoirs to compute the current I_α into reservoir α as

$$I_\alpha = \int \left[f_\alpha(\epsilon) \frac{\mathrm{d}}{\mathrm{d}\epsilon} \left(I^{\alpha \to \alpha} \right) + \sum_{\beta \neq \alpha} f_\beta(\epsilon) \frac{\mathrm{d}}{\mathrm{d}\epsilon} \left(I^{\beta \to \alpha} \right) \right] \mathrm{d}\epsilon.$$

To determine the functions $\frac{\mathrm{d}}{\mathrm{d}\epsilon} I^{\alpha \to \beta}(\epsilon)$ and $\frac{\mathrm{d}}{\mathrm{d}\epsilon} I^{\alpha \to \alpha}(\epsilon)$ (that is, the current densities with respect to energy), we compute the differentials of the current contributions as the probability current per k multiplied by the electron charge. In symbols we have, using (2.1.3),

$$\begin{aligned} \mathrm{d}I^{\alpha \to \alpha} &= -e\mathrm{d}J^{\alpha \to \alpha} = -ej^{\alpha \to \alpha}(k)\mathrm{d}k, \\ &= -e\frac{\hbar}{2mi} \left(\langle n, \alpha | \psi_{\alpha,k} \rangle^* \partial_n \left[\langle n, \alpha | \psi_{\alpha,k} \rangle \right] - \text{c.c.} \right) \mathrm{d}k, \\ &= \frac{e\hbar k}{2\pi m} \left(1 - |R_\alpha(k)|^2 \right) \mathrm{d}k, \\ &= \frac{e}{h} \left(1 - |R_\alpha(\epsilon)|^2 \right) \mathrm{d}\epsilon. \end{aligned}$$

---

[16]Hence the name, as we treat it as a point, which has no internal structure.

Similarly,

$$\mathrm{d}I^{\alpha\to\beta} = -\frac{e}{h}|T_{\alpha,\beta}(\epsilon)|^2\mathrm{d}\epsilon.$$

Plugging this into our integral and using (4.0.2) and (4.0.3) we find the *Landauer-Büttiker formula*

$$I_\alpha = \frac{e}{h}\int \mathrm{d}\epsilon \left\{ \sum_{\beta\neq\alpha} |T_{\alpha,\beta}(\epsilon)|^2 \left(f_\alpha(\epsilon) - f_\beta(\epsilon)\right) \right\}, \qquad (4.0.4)$$

whose power lies in the fact that it has completely separated the general macroscopic statistical physics from the microscopic details of the particular system under consideration.

The groundwork for this equation was laid by Rolf Landauer[17] and Markus Büttiker[18] in their individual 1957 and 1986 papers [11] and [5] (see equation (2)) respectively. It has proven to be invaluable in the study of multi-terminal mesoscopic devices (see [3]), and has inspired many attempts at generalisations to more sophisticated models (see chapter 8).

If we take the limit of 0 temperature, (4.0.4) simplifies to (assuming $\mu_\alpha > \mu_\beta \ \forall\beta$)

$$I_\alpha = \frac{e}{h}\sum_{\beta\neq\alpha}\int_{\mu_\beta}^{\mu_\alpha} |T_{\alpha,\beta}(\epsilon)|^2\mathrm{d}\epsilon, \qquad (4.0.5)$$

which is even more intuitive than (4.0.4). From the formula one sees that the current consists of an integral over the electrons that have the proper wavenumbers to participate in transport (i.e. they are available in reservoir β, and reservoir α has room for them) multiplied by their probability to make it to reservoir α (see also the cartoon in fig.4.1).
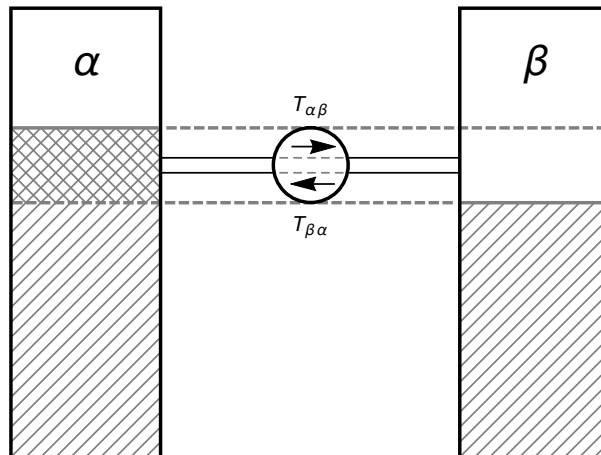
Figure 4.1: A cartoon of the situation described in this section, for $T = 0$.

---

[17]German-American, 1927-1999.
[18]Swiss, 1950-2013.

Assuming we have two reservoirs L and R and Taylor expanding to leading order in the chemical potential bias $\mu_{L/R} = \mu \pm eV/2$ one finds for the linear (DC) conductance

$$G := \frac{\mathrm{d}I}{\mathrm{d}V} = \frac{e^2}{h}|T_{L,R}(\mu)|^2. \tag{4.0.6}$$

Note the appearance of the famous *conductance quantum* e^2/h. However the transmission need not be an integer, so there is no sign of conductance quantisation in this model, but one conductance quantum is still the maximal conductance for the point contact we are considering here.

Now we need to compute the coefficients of the plane waves, which we shall tackle in the next section.

5 A Green Function Approach to the Transmission and Reflection Coefficients

5.1 The Lippmann-Schwinger Equation

We begin by writing our Hamiltonian as $H =: H_0 + H_t =: H_0 + V$, then we want to solve

$$(H_0 + V) \left| \psi_{\alpha,k} \right\rangle = E_k \left| \psi_{\alpha,k} \right\rangle .$$

To do this we make the scattering Ansatz (compare to (4.0.1)) $\psi_{\alpha,k} = \psi_{\alpha,k}^0 + \psi_{\alpha,k}^s$, where we assume that $H_0 \psi_{\alpha,k}^0 = E_k \psi_{\alpha,k}^0$. In general this is quite a strong assumption (note that all three wavefunctions involved are indexed by the same quantum numbers) and is not always meaningful, but it is possibly exact (as it is for our case) and not a perturbation theory approach. However, in our case we have assumed elastic scattering, and additionally the scattered contributions have to respect the dispersion of the wire. In other words, we can only consider energies E_k that are contained in the cosine-band, where we can always find a matching eigenfunction. One can now rewrite the problem as follows

$$V \left| \psi_{\alpha,k} \right\rangle = (E_k - H_0) \left[\left| \psi_{\alpha,k}^0 \right\rangle + \left| \psi_{\alpha,k}^s \right\rangle \right] = (E_k - H_0) \left| \psi_{\alpha,k}^s \right\rangle .$$

This motivates us to investigate the formal expression

$$\left| \psi_{\alpha,k} \right\rangle = \left| \psi_{\alpha,k}^0 \right\rangle + \left| \psi_{\alpha,k}^s \right\rangle = \left| \psi_{\alpha,k}^0 \right\rangle + \frac{1}{E_k - H_0} V \left| \psi_{\alpha,k} \right\rangle .$$

Clearly this is not well defined, as $E_k - H_0$ has non-trivial kernel, and in general differential operators are not uniquely invertible if no boundary conditions are imposed. A way to fix this is to add an infinitesimal imaginary part $\pm i 0^+ =: \pm i\eta$ in the denominator, which will turn out to be justified later. This gives rise to the *Lippmann-Schwinger equation*

$$\left| \psi_{\alpha,k}^\pm \right\rangle = \left| \psi_{\alpha,k}^0 \right\rangle + \frac{1}{E_k - H_0 \pm i\eta} V \left| \psi_{\alpha,k}^\pm \right\rangle ,$$

named after Bernard Lippmann[19] and his doctoral advisor Julian Schwinger[20], who introduced it in their 1950 paper [13][21].

Using the operator identity

$$\frac{1}{A - B} = \frac{1}{A} + \frac{1}{A} B \frac{1}{A - B}, \tag{5.1.1}$$

which may be readily proven by simply multiplying by $A - B$ on either the left or the right, we can express this equation more conveniently[22] as

$$\left| \psi_{\alpha,k}^\pm \right\rangle = \left| \psi_{\alpha,k}^0 \right\rangle + \frac{1}{E_k - H \pm i\eta} V \left| \psi_{\alpha,k}^0 \right\rangle . \tag{5.1.2}$$

---

[19] American, 1914-1988.

[20] also American, 1918-1994, awarded the 1965 Nobel prize for physics together with Richard Feynman (American, 1918-1988) and Sin-Itiro Tomonaga (Japanese, 1906-1979) for their work on quantum electrodynamics.

[21] It is interesting to note that this approach pre-dates the one due to Landauer and Büttiker.

[22] The word convenient is relative, we get rid of the recursion but we get back a harder operator to invert. This is a prime example of Rembert Duine's (Dutch, 1975-) *"wet van behoud van elende"*.

In our case, $\left\langle n, \beta \middle| \psi^0_{\alpha,k} \right\rangle = 0$ ($\beta \neq \alpha$), and $\left\langle n, \alpha \middle| \psi^0_{\alpha,k} \right\rangle = -i\sqrt{2/\pi} \sin(kn)$. The first equality comes from our assumption that the reservoirs are isolated, and the second uses the sin because of the boundary condition that the wave function vanishes at $n = 0$, and the factor $-i$ is chosen for convenience.

We now multiply (5.1.2) with the bra $\langle n, \beta|$ to find

$$
\begin{aligned}
\langle n, \beta | \psi_{\alpha,k} \rangle &= \langle n, \beta | \psi^0_{\alpha,k} \rangle + \left\langle n, \beta \middle| \frac{1}{E_k - H + i\eta} H_t \middle| \psi^0_{\alpha,k} \right\rangle, \\
&= -t_\alpha \left\langle n, \beta \middle| \frac{1}{E_k - H + i\eta} \middle| 0, \alpha \right\rangle \langle 1, \alpha | \psi^0_{\alpha,k} \rangle, \\
&= it_\alpha \sqrt{\frac{2}{\pi}} \sin(k) \left\langle n, \beta \middle| \frac{1}{E_k - H + i\eta} \middle| 0, \alpha \right\rangle,
\end{aligned}
$$

where we have used the expression (compare to (3.0.4))

$$
H_t = -\sum_{\beta'} t_{\beta'} \left(|0, \beta'\rangle \langle 1, \beta'| + |1, \beta'\rangle \langle 0, \beta'| \right). \tag{5.1.3}
$$

We now revert the identity (5.1.1), which yields

$$
\begin{aligned}
\langle n, \beta | \psi_{\alpha,k} \rangle = it_\alpha \sqrt{\frac{2}{\pi}} \sin(k) &\left(\left\langle n, \beta \middle| \frac{1}{E_k - H_0 + i\eta} \middle| 0, \alpha \right\rangle, \right. \\
&\left. + \left\langle n, \beta \middle| \frac{1}{E_k - H_0 + i\eta} H_t^\beta \frac{1}{E_k - H + i\eta} \middle| 0, \alpha \right\rangle \right).
\end{aligned}
$$

The first term vanishes, as the resolvent does not induce any transitions from reservoir α to reservoir β. In the second term we can simplify the sandwiched operator by first noting that the tunnel Hamiltonian will move the state out of the dot system and into reservoir β, so H_0 becomes just H_r^β. After also inserting our expression (5.1.3) for H_t^β, the result can be written

$$
\begin{aligned}
\langle n, \beta | \psi_{\alpha,k} \rangle &= -it_\alpha t_\beta \sqrt{\frac{2}{\pi}} \sin(k) \left\langle n, \beta \middle| \frac{1}{E_k - H_r^\beta + i\eta} \middle| 1, \beta \right\rangle \left\langle 0, \beta \middle| \frac{1}{E_k - H + i\eta} \middle| 0, \alpha \right\rangle, \\
&:= i\sqrt{\frac{2}{\pi}} \frac{t_\alpha t_\beta}{t} \sin(k) e^{ikn} \langle 0, \beta | G^R(E_k) | 0, \alpha \rangle, \tag{5.1.4}
\end{aligned}
$$

where in the last line we have used the result

$$
\left\langle n, \beta \middle| \frac{1}{\epsilon_k - H_{\text{res}}^\beta + i\eta} \middle| 1, \beta \right\rangle = -\frac{e^{ikn}}{t},
$$

which is derived in appendix A, and we have defined

$$
G^{R/A}(E_k) := \frac{1}{E_k - H \pm i\eta}. \tag{5.1.5}
$$

If we now compare (5.1.4) with our plane wave Ansatz (4.0.1), we see that

$$
T_{\beta,\alpha}(E_k) = 2i \sin(k) \frac{t_\alpha t_\beta}{t} \langle 0, \beta | G^R(E_k) | 0, \alpha \rangle. \tag{5.1.6}
$$

We now repeat this recipe to find the reflection coefficient,

$$\langle n, \alpha | \psi_{\alpha,k} \rangle = \langle n, \alpha | \psi_{\alpha,k}^0 \rangle + \left\langle n, \alpha \left| \frac{1}{E_k - H + i\eta} H_t^\alpha \right| \psi_{\alpha,k}^0 \right\rangle,$$

only now the first term does not vanish. We insert our expression for H_t^α, play our game with (5.1.1), and cancel terms with the same logic as before, which results in

$$\langle n, \alpha | \psi_{\alpha,k} \rangle = -i\sqrt{\frac{2}{\pi}} \sin(nk) + i\sqrt{\frac{2}{\pi}} \frac{t_\alpha^2}{t} \sin(k) e^{ikn} \left\langle 0, \alpha \left| G^R(E_k) \right| 0, \alpha \right\rangle.$$

Comparing this again to (4.0.1) now gives us

$$R_\alpha(E_k) = 2i \sin(k) \frac{t_\alpha^2}{t} \left\langle 0, \alpha \left| G^R(E_k) \right| 0, \alpha \right\rangle - 1. \tag{5.1.7}$$

5.2 A Note on Green Functions

The operators defined in (5.1.5) are called the *retarded* and *advanced Green function* respectively. Keep in mind that despite their names they are not functions. Moreover, they are not what a mathematician would call or a classical physicist would have called a Green function. Green functions were originally introduced by mathematical physicist George Green[23] in an 1828 paper on his mathematical formulation of electromagnetism. He used it to solve Poisson's[24] differential equation for the electric field, deriving the now well known integral expressions for the electric potential. In mathematical terms, given a differential operator $L(x)$, a Green function for L is a "function" that satisfies

$$L(x)G(x, x') = \delta(x - x'),$$

i.e. the response of the system to a unit excitation at x'. This is useful since once we have the Green function, we can solve any inhomogeneous problem $L(x)f = g$ via

$$L(x) \int G(x, x')g(x')\mathrm{d}x' = \int \delta(x - x')g(x')\mathrm{d}x' = g(x).$$

So in a sense, the Green function inverts the operator L. It is because of this property that we call (5.1.5) Green functions, as these are in a sense inverses of the Hamiltonian. Since we usually sandwich $G^{R/A}$ between the states $|0, \alpha\rangle$ and $|0, \beta\rangle$ and the result is related to transmission and reflection, it can also be thought of as a *propagator* of our system, i.e. given the "excitation" $|0, \alpha\rangle$ to what extent does it "propagate" to the states $|0, \beta\rangle$ (note however that a proper propagator also takes into account the times at which the measurements are made). The simplest concrete example of a propagator is the case of the free one dimensional particle, where we can write

$$G(x, t; x', t') = \frac{1}{i\hbar} \theta(t - t') \left\langle x \left| \exp\left(-\frac{i}{\hbar}(t - t')H \right) \right| x' \right\rangle,$$

---

[23]British, 1793-1841, also known for Green theorem.
[24]French, 1781-1840, known for lots of things.

where θ is the Heaviside step function. One can evaluate the matrix element as follows

$$\left\langle x \left| \exp\left(-\frac{i}{\hbar}(t-t')H\right) \right| x' \right\rangle = \int \mathrm{d}k\mathrm{d}k' \left\{ \langle x|k\rangle \left\langle k \left| \exp\left(\frac{i\hbar\partial_x^2}{2m}(t-t')\right) \right| k' \right\rangle \langle x'|k'\rangle \right\},$$

$$= \frac{1}{2\pi} \int \mathrm{d}k \left\{ \exp\left(ik(x-x') - \frac{i\hbar k^2}{2m}(t-t') \right) \right\},$$

$$= \sqrt{\frac{m}{2\pi\hbar i t}} \exp\left\{ -\frac{m(x-x')^2}{2i\hbar(t-t')} \right\},$$

where the last step can be obtained by completing the square in the exponent and then using a standard Gaußian integral. In conclusion, the (retarded) free particle propagator in one dimension is given by

$$G(\Delta x; \Delta t) = \frac{1}{i\hbar}\theta(\Delta t)\sqrt{\frac{m}{2\pi\hbar i t}} \exp\left\{ -\frac{m\Delta x^2}{2i\hbar\Delta t} \right\}.$$

5.3 The Dyson equation, Self Energy, and Effective Broadening

The next step in our derivation is to compute the matrix elements

$$\left\langle 0, \beta \left| G^{R/A}(E_k) \right| 0, \alpha \right\rangle.$$

To find them we consider the states $|a\rangle$, $|b\rangle$ of the dot system and once again dance around with (5.1.1),

$$G_{a,b}^R(E_k) := \left\langle a \left| \frac{1}{E_k - H + i\eta} \right| b \right\rangle,$$

$$= \left\langle a \left| \frac{1}{E_k - H_d + i\eta} + \frac{1}{E_k - H_0 + i\eta} H_t \frac{1}{E_k - H + i\eta} \right| b \right\rangle,$$

$$= \left\langle a \left| \frac{1}{E_k - H_d + i\eta} \right| b \right\rangle + \left\langle a \left| \frac{1}{E_k - H_0 + i\eta} H_t \frac{1}{E_k - H_0 + i\eta} \right| b \right\rangle,$$

$$+ \left\langle a \left| \frac{1}{E_k - H_0 + i\eta} H_t \frac{1}{E_k - H_0 + i\eta} H_t \frac{1}{E_k - H + i\eta} \right| b \right\rangle.$$

Recall that the tunnel operator only ever moves states out of the dot system into a reservoir or the other way around. This means that since we consider only states in the dot, the term involving only one instance of H_t is zero, and in the term containing H_t twice, only terms involving the same reservoir will remain. We also introduce some new objects, namely the *local Green functions* for the dot and the reservoirs, which we denote

$$g^{R/A}(E_k) = \frac{1}{E_k - H_d \pm i\eta}, \quad g_\alpha^{R/A}(E_k) = \frac{1}{E_k - H_r^\alpha \pm i\eta}. \tag{5.3.1}$$

Note that we can write (5.1.4) with this notation as

$$\left\langle n, \beta \left| g_\beta^R(E_k) \right| 1, \beta \right\rangle = -\frac{1}{t}e^{ikn}, \tag{5.3.2}$$

so in fact we already computed the 1st "column" of the local reservoir Green function. With this, the result of our computation above reduces to

$$G_{a,b}^R(E_k) = \langle a|g^R(E_k)|b\rangle + \left\langle a\middle| g^R(E_k) \left[\sum_\alpha H_t^\alpha g_\alpha^R(E_k) H_t^\alpha\right] G^R(E_k) \middle| b\right\rangle.$$

Now, what else is there to do but introduce more notation? This time we define the so called *self-energy* as the object in square brackets in the previous equation, explicitly

$$\Sigma^{R/A}(E_k) = \sum_\alpha H_t^\alpha g_\alpha^{R/A}(E_k) H_t^\alpha. \tag{5.3.3}$$

Similarly to the Green functions, we have that $\left(\Sigma^{R/A}\right)^\dagger = \Sigma^{A/R}$. Using all of our fancy new notation and keeping in the back of our minds that we work exclusively in the dot, we drop the bras and kets to find the *Dyson equation*[25]

$$G^R = g^R + g^R \Sigma^R G^R. \tag{5.3.4}$$

Iterating (5.3.4) yields

$$G^R = g^R + g^R \Sigma^R g^R + g^R \Sigma^R g^R \Sigma^R g^R + \cdots,$$
$$= \left(\text{id} + g^R \Sigma^R + \left(g^R \Sigma^R\right)^2 + \cdots\right) g^R.$$

We recognize the right hand side as the Neumann[26] series, whose result is analogous to the geometric series. Thus we have

$$G^R = \frac{1}{1 - g^R \Sigma^R} g^R = \frac{1}{(g^R)^{-1} - \Sigma} = \frac{1}{E_k - H_d - \Sigma(E_k)}.$$

One can repeat this scheme for the advanced Green function as well to find for the global Green function restricted to the dot system

$$G^{R/A}(E_k) = \frac{1}{E_k - H_d - \Sigma^{R/A}}. \tag{5.3.5}$$

A striking feature of this result is that our infinitesimal imaginary term appears to have vanished, but this is not entirely true, it has hidden itself in our definition of the self-energy. However, one should note that the self-energy generates a finite imaginary part by itself that is independent of the convergence factor we introduced earlier. Additionally, the self-energy has a physical meaning that is independent of our particular definition. It represents the contribution to the energy of an excitation due to interactions with the system it is a part of, and is frequently used to define some form of effective mass for a (quasi-)particle. Thus the real and imaginary parts of Σ contain information about these excitations. The real part represents a shift in resonance and can be used to find an expression for the aforementioned effective mass. The imaginary part of Σ can be interpreted as a decay rate for the excitation when one keeps in mind the unitary time evolution operator $\exp\left\{-\frac{i}{\hbar}tH\right\}$. Thus it makes

---

[25]named after Freeman Dyson (American, 1923-), who is also known for the Dyson series, which represents a formal solution to the time-dependent Schrödinger equation, and in popular culture for the concept of the Dyson sphere.

[26]After Carl Neumann (German, 1832-1925).

sense to define an *effective broadening* (note the similarity to taking the imaginary part of a complex number)

$$\Gamma = i(\Sigma^R - \Sigma^A), \tag{5.3.6}$$

which is obviously self-adjoint. A useful identity involving this broadening is

$$G^R - G^A = -iG^R\Gamma G^A = -iG^A\Gamma G^R, \tag{5.3.7}$$

which one can prove as follows,

$$
\begin{aligned}
G^R - G^A &= G^R \frac{1}{G^A} G^A - G^R \frac{1}{G^R} G^A = G^R \left(\frac{1}{G^A} - \frac{1}{G^R} \right) G^A, \\
&= G^R \left(E_k - H_d - \Sigma^A - E_k + H_d + \Sigma^R \right) G^A, \\
&= (-i)iG^R \left(\Sigma^R - \Sigma^A \right) G^A = -iG^R\Gamma G^A.
\end{aligned}
$$

The second equality in (5.3.7) is obtained by taking Hermitian conjugates. Coming back to the self-energies, for our system we can explicitly compute them as

$$\Sigma^{R/A} = \sum_\alpha t_\alpha^2 \langle 1,\alpha | g_\alpha^R | 1,\alpha \rangle |0,\alpha\rangle \langle 0,\alpha| = -\frac{1}{t} e^{\pm ik} \sum_\alpha t_\alpha^2 |0,\alpha\rangle \langle 0,\alpha|. \tag{5.3.8}$$

We can use this to also obtain the broadening

$$\Gamma(E_k) = \frac{1}{2}\sin(k) \sum_\alpha t_\alpha^2 |0,\alpha\rangle \langle 0,\alpha| =: \sum_\alpha \Gamma_\alpha(E_k). \tag{5.3.9}$$

This now gives us everything we need to compute the operator $E_k - H_d - \Sigma^R$ and invert it to find the retarded Green function.

Finally we present a formal proof of the identities (4.0.2) and (4.0.3). We begin by computing

$$
\begin{aligned}
|T_{\beta,\alpha}|^2 &= 4\sin^2(k) \frac{t_\alpha^2 t_\beta^2}{t^2} \left| \langle 0,\beta | G^R | 0,\alpha \rangle \right|^2, \\
&= \langle 0,\beta | \Gamma_\beta | 0,\beta \rangle \langle 0,\beta | G^R | 0,\alpha \rangle \langle 0,\alpha | \Gamma_\alpha | 0,\alpha \rangle \langle 0,\alpha | G^A | 0,\beta \rangle, \\
&= \langle 0,\beta | \Gamma_\beta G^R \Gamma_\alpha G^A | 0,\beta \rangle.
\end{aligned}
$$

Notice now that $\langle 0,\beta' | \Gamma_\beta = 0$ for any $\beta' \neq \beta$, which allows us to write

$$|T_{\beta,\alpha}|^2 = \mathrm{Tr}\left(\Gamma_\beta G^R \Gamma_\alpha G^A \right). \tag{5.3.10}$$

We can now exploit (5.3.7) and the fact that the trace is invariant under cyclic permutations ($\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$) and linear to show (4.0.3),

$$
\begin{aligned}
\sum |T_{\beta,\alpha}|^2 &= \mathrm{Tr}\left(\Gamma G^R \Gamma_\alpha G^A \right) - \mathrm{Tr}\left(\Gamma_\alpha G^R \Gamma_\alpha G^A \right), \\
&= \mathrm{Tr}\left(\Gamma_\alpha G^A \Gamma G^R \right) - \mathrm{Tr}\left(\Gamma_\alpha G^R \Gamma_\alpha G^A, \right) \\
&= \mathrm{Tr}\left(\Gamma_\alpha G^R \Gamma G^A \right) - \mathrm{Tr}\left(\Gamma_\alpha G^R \Gamma_\alpha G^A \right), \\
&= \sum \mathrm{Tr}\left(\Gamma_\alpha G^R \Gamma_\beta G^A \right) = \sum |T_{\alpha,\beta}|^2.
\end{aligned}
$$

We also compute

$$
\begin{aligned}
|R_\alpha|^2 &= 1 + 4\sin^2(k) \frac{t_\alpha^4}{t^2} \left| \langle 0,\alpha | G^R | 0,\alpha \rangle \right|^2 + 2\sin(k) \frac{t_\alpha^2}{t} \langle 0,\alpha | i \left(G^A - G^R \right) | 0,\alpha \rangle, \\
&= 1 + \mathrm{Tr}\left(\Gamma_\alpha G^R \Gamma_\alpha G^A \right) - \mathrm{Tr}\left(\Gamma_\alpha G^R \Gamma G^A \right),
\end{aligned}
$$

which immediately implies (4.0.2) when paired with the third line from the previous computation.

6 Proof of Concept: a Single Impurity

We consider the case of a single site system with energy ϵ connected to two reservoirs, and tunnelling amplitude t' on both sides. Thus we have

$$H_d + H_t = \epsilon \, |s\rangle \, \langle s| - t' \left[|L,1\rangle \, \langle s| + |R,1\rangle \, \langle s| + \text{h.c.} \right],$$

where have denoted the occupied state of the dot as $|s\rangle$. This system is easy to treat since the Hilbert space of the dot is one dimensional, and hence inverting operators is trivial. The first step is to compute the only matrix element of $G^{R/A}$, which is simply the function

$$\langle s| \, G^{R/A} \, |s\rangle = \frac{1}{\omega - \epsilon - \langle s| \, \Sigma^{R/A} \, |s\rangle}.$$

For convenience we will make no notational distinction between $\langle s| \hat{O} |s\rangle$ and $\hat{O}$ itself in the rest of the section. It is a straightforward procedure to use (5.3.8) and (5.3.9) to find
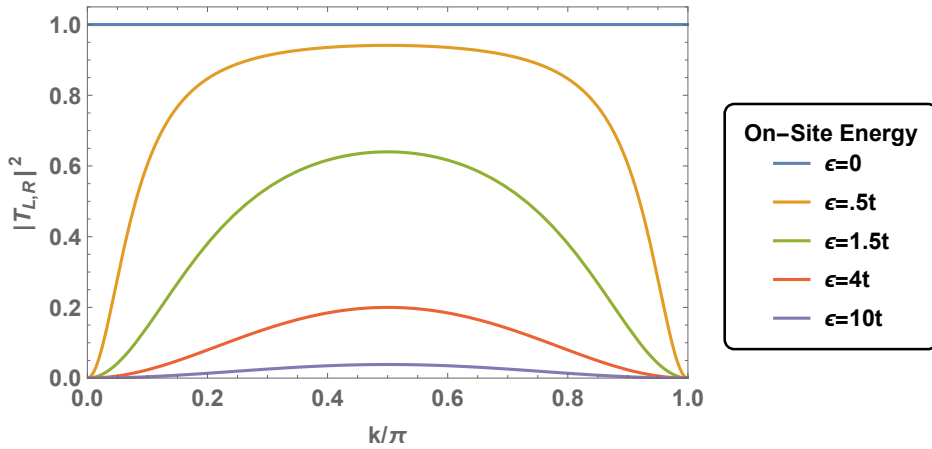
$$\Sigma^{R/A} = -2\frac{(t')^2}{t} e^{\pm ik}, \ \ \Gamma_{L/R} = -2\frac{(t')^2}{t}\sin(k), \ \ \Gamma = -4\frac{(t')^2}{t}\sin(k), \tag{6.0.1}$$
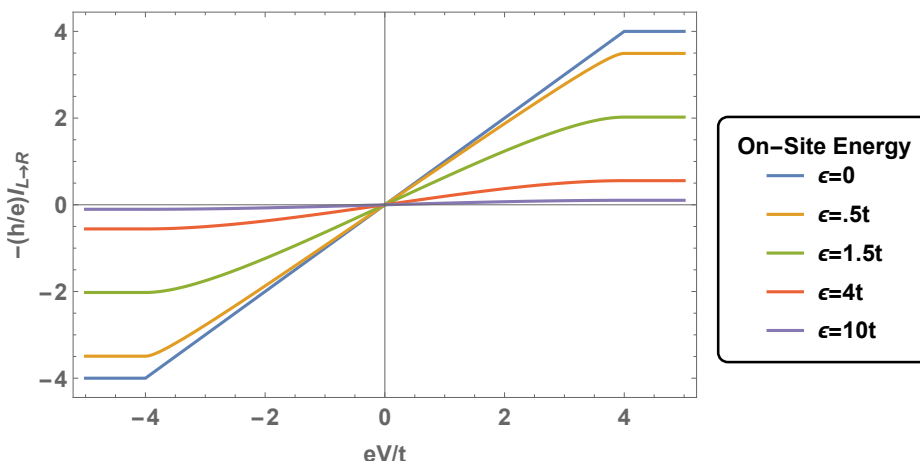
which allows us to write

$$\Sigma^{R/A} = \mathfrak{Re}\left[\Sigma^R\right] \mp \frac{i}{2}\Gamma.$$

We use now the derivation of (5.3.10) to compute

$$|T_{L,R}(\omega)|^2 = \Gamma_L \Gamma_R G^A G^R = \Gamma_L \Gamma_R \frac{1}{\omega - \epsilon - \mathfrak{Re}\left[\Sigma^R\right] + \frac{i}{2}\Gamma} \frac{1}{\omega - \epsilon - \mathfrak{Re}\left[\Sigma^R\right] - \frac{i}{2}\Gamma},$$

$$= 2\pi \frac{\Gamma_L(\omega)\Gamma_R(\omega)}{\Gamma(\omega)} \frac{1}{\pi} \frac{\frac{1}{2}\Gamma(\omega)}{(\omega - \epsilon - \mathfrak{Re}\left[\Sigma^R(\omega)\right])^2 + (\frac{1}{2}\Gamma(\omega))^2}, \tag{6.0.2}$$

Figure 6.1: A plot of the transmission $(6.0.3)$ as a function of k in the limit of equal coupling $(t' = t)$ for several values of ϵ. Note that transmission is perfect for $\epsilon = 0$ and decays overall for larger values, as one would expect.

22

Figure 6.2: A plot of the current versus bias in the equal coupling limit obtained by numerically integrating (6.0.3) according to (4.0.4) at 0 temperature for the same values of ϵ as in fig.6.1. Note the levelling out of the current for biases larger than $4t$, this is due to the finite bandwidth of the cosine band (which is exactly $4t$). For the particular case of $\epsilon = 0$ we see that the current is linear and behaves in accordance with $I = GV$, (see (4.0.6)).

which has the form of a Lorentzian[27] (more commonly known as the Cauchy distribution outside physics) of width $\Gamma/2$ centred at $\epsilon + \mathfrak{Re}\left[\Sigma^R\right]$, reinforcing our earlier discussion of these quantities. If we now substitute the expressions (6.0.1) into (6.0.2) we arrive at the explicit form

$$|T_{L,R}(\omega)|^2 = \frac{4\sin^2(k)\frac{(t')^4}{t^2}}{\left(\omega - \epsilon - 2\cos(k)\frac{(t')^2}{t}\right)^2 + 4\sin^2(k)\frac{(t')^4}{t^2}},$$

where one should keep in mind that k and ω are related by $\omega = -2t\cos(k)$. We will consider two cases in detail, the first being $t = t'$ and the second the wide-band limit $(t \gg t')$.

Setting $t = t'$, if we substitute the dispersion relation into the above formula, something peculiar happens,

$$|T_{L,R}(k)|^2 = \frac{(2t\sin(k))^2}{\epsilon^2 + (2t\sin(k))^2} = \left[1 + \left(\frac{\epsilon}{2t\sin(k)}\right)^2\right]^{-1}, \qquad (6.0.3)$$

which is plotted in fig.6.1. Notice that the peak of the transmission always occurs for $k = \pi/2$, independently of the value of ϵ. This is quite strange, as one would expect ϵ to behave like a threshold, below which very little current is transmitted, but this is not the case (see fig.6.2). Instead we see that the current behaves linearly for small bias and that for $V = \pm 4t$ it becomes constant, as the band is full. Increasing the barier strength ϵ seems to only decrease the magnitude of the current and smoothen out the profile, which makes sense as the variations on the bias scale are then small compared to the barier strength.

However, one could argue that it is indeed correct as follows. It is a canonical exercise in any introductory quantum mechanics course to compute the transmission

---

[27]After Hendrik Lorentz (Dutch, 1853-1928), awarded the 1902 Nobel prize together with fellow Dutchman Pieter Zeeman (1865-1943) for discovering and explaining the Zeeman effect. Also well known for laying part of the mathematical framework of special relativity.
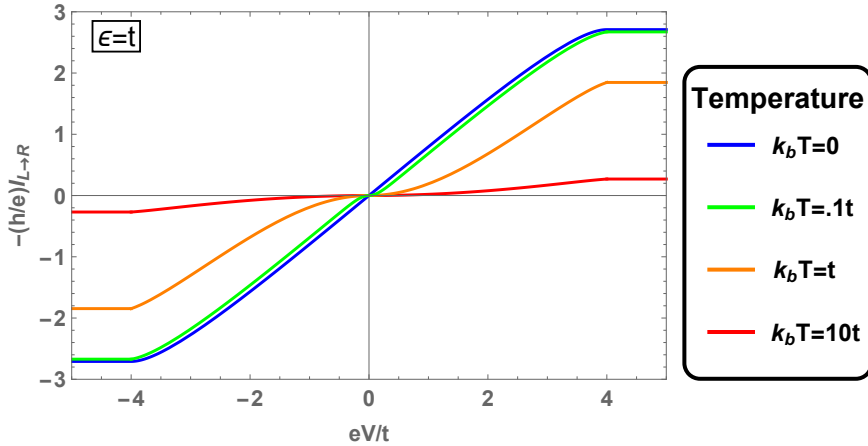
Figure 6.3: A plot of the current versus bias in the equal coupling limit obtained by numerically integrating (6.0.3) according to (4.0.4) for a range of temperatures and the fixed value $\epsilon = t$ (compare to fig.6.2). From blue to red we have $k_b T = 0$, $0.1t$, t, $10t$. From this image on could conclude that thermalisation very quickly destroys the special properties of the system that we have discussed so far.

coefficient for a delta-function potential with strength ϵ. This is essentially the same system as we have here, a single long wire with an impurity. One can use the plane wave Ansatz (4.0.1) and the boundary conditions to the Schrödinger equation (2.1.4) to derive

$$\overline{T}(\omega) = \frac{1}{1 + \frac{\epsilon^2 m}{2\hbar^2 \omega}}, \qquad (6.0.4)$$

where $\omega(k) = \hbar^2 k^2 / 2m$ is the free electron dispersion. Using the definition of velocity $v(k) = \partial_k \omega(k)$ one can rewrite this as

$$\overline{T}(k) = \left[1 + \left(\frac{\epsilon}{v(k)} \right)^2 \right]^{-1},$$

which reproduces both (6.0.3) and (6.0.4) when the relevant dispersion is chosen. Besides supporting the claim that our result is correct, this suggests that in this regime the important quantity is not energy, but velocity. We can now explain the behaviour of our result for the transmission coefficient as a peculiarity of the cosine-band, since the velocity is always maximal about $\omega = 0$ or equivalently $k = \pi/2$ for this dispersion relation.

On the other hand the effects of temperature (seen in fig.6.3) are what one would expect. At low temperatures we see the same overal profile but with slightly reduced magnitude, this happens because as soon as temperature is finite the fermi-distributions in (4.0.4) are no longer step functions and hence it becomes less likely to have an electron available on the left and less likely to have an available state for it on the right. This effect only becomes stronger for higher temperatures, but it also comes into play that we have centered our bias at the transimission maximum, meaning that even though thermalisation allows a larger portion of the band to participate, these states are less likely to be transmitted.

We now consider the wide-band limit, i.e. $t \gg t'$. From (6.0.2) and (6.0.1) we expect to see very narrow peaks (Lorentzians even tend to delta functions in the limit of
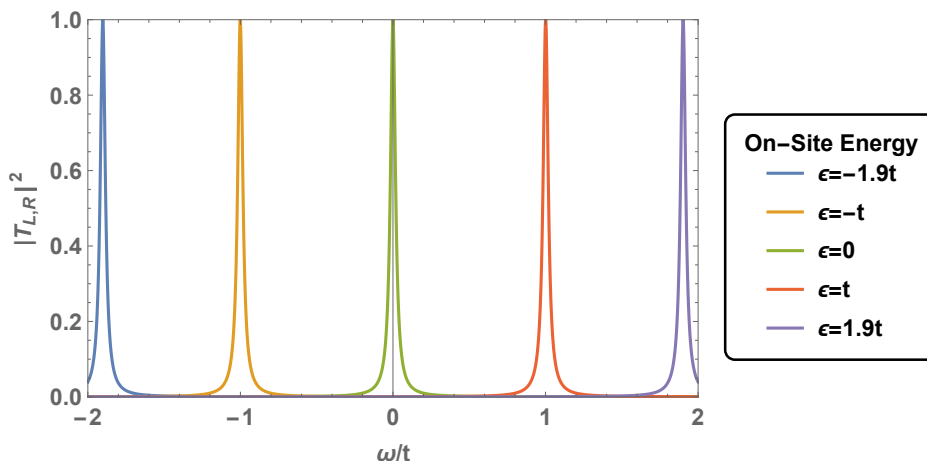
Figure 6.4: A plot of the transmission (6.0.2) as a function of energy for several values of epsilon, in the wideband limit ($10t' = t$). Since the effective broadening Γ is proportional to t' and the transmission function is a Lorentzian, we expect to see delta-function like transmission centred at the relevant value of ϵ, and this is indeed the case.

vanishing width) centered approximately around ϵ, as the self energy is also very small (conversely we saw in fig.6.1 that the width was compareable to the band size for the case of equal hopping amplitudes). Looking at fig.6.4, that is indeed what we see. For the current an exact result was can be found in [1] (equation (63)) with which we compare our results,

$$I_{\text{st}} = \frac{1}{\pi} \frac{\Gamma'_L \Gamma'_R}{\Gamma'} \left(\arctan\left(\frac{V/2 - \epsilon}{\Gamma'/2} \right) + \arctan\left(\frac{V/2 + \epsilon}{\Gamma'/2} \right) \right), \qquad (6.0.5)$$

where $\Gamma'_{R/L} = 2\pi(t')^2$ and $\Gamma' = \Gamma'_L + \Gamma'_R$. As can be seen from fig.6.5, the results are in excellent agreement, even though the exact result was derived using very different methods.

Note that this time we observe exactly what we expected to see earlier in this section. There is a small amount of current even at low bias due to tunnelling, and as soon as the barrier strength is reached the current rises sharply until it fills the band. The band width is now much less since the system is bottlenecked at the quantum dot in this limit, hence the current essentially vanishes altogether when the barrier strength exceeds the band width of the dot. Qualitatively one can see that the overall magnitude of the current is about a factor 100 smaller than before. This is due to the fact that we chose $t/t' = 10$ and $t' = 1$ in our computations, and the inverse square of this ratio is present in the prefactor of (6.0.2). A plot of the effects of finite temperature can be found in fig.6.6, which exhibits behaviour that is very similar to the previous case, with the only major difference being the fact that the onset of the current happens more steeply, which is due to the thermal broadening effects described before, only this time there is much to gain from this broadening at first as the current feels the transmission peak earlier, albeit at a reduced strength ($|f_L(\omega) - f_R(\omega)| \leq 1$).
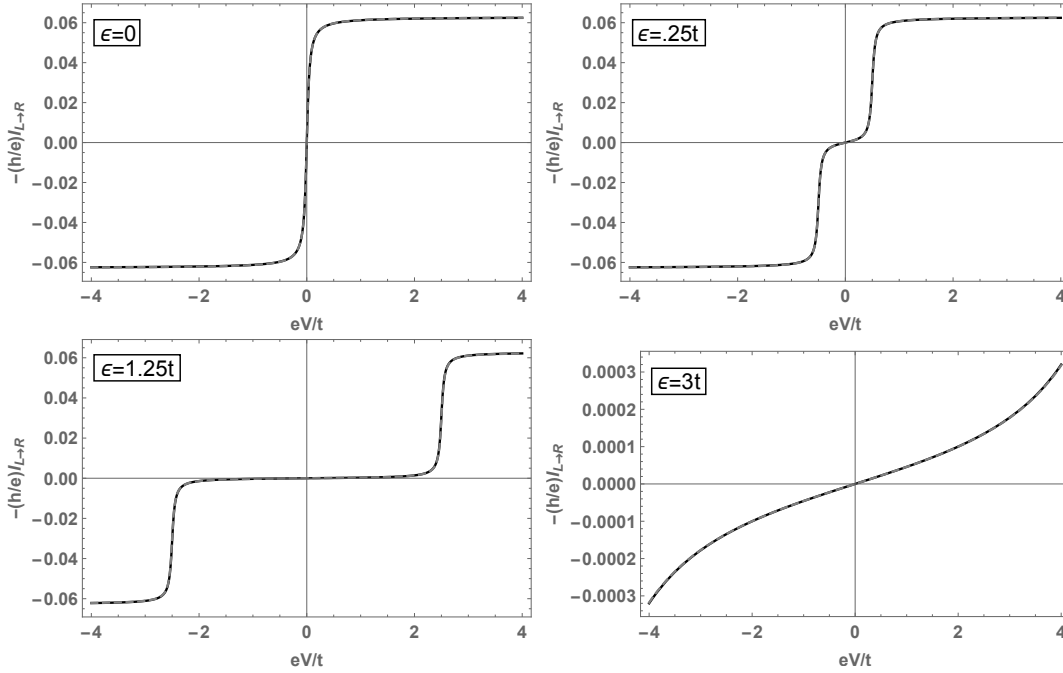
Figure 6.5: A plot of the current versus bias in the wideband limit obtained by numerically integrating $(6.0.2)$ according to $(4.0.4)$ at 0 temperature (in dashed black) together with the exact result $(6.0.5)$ (in gray) at 0 temperature for several values of ϵ. Clockwise: $\epsilon = 0, \ 0.25t, \ 3t, \ 1.25t$. Visually, there seems to be no discernible deviations. Note the scale of the ordinate in the bottom right graph, here the on-site energy is larger than the bandwidth and practically no current flows.
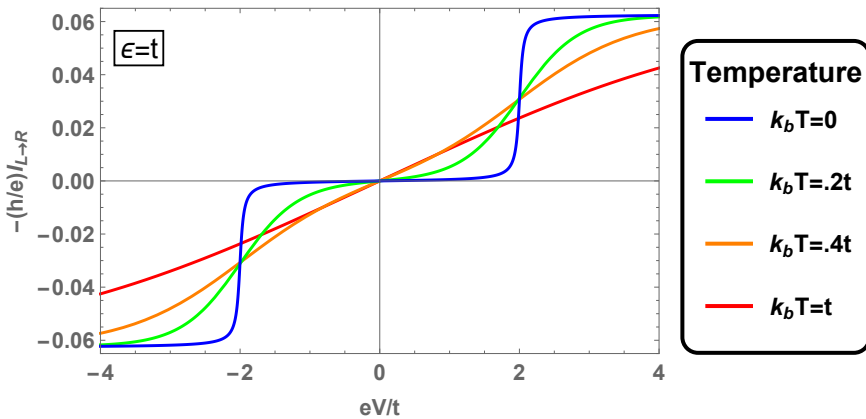
Figure 6.6: The numerically integrated current versus from fig.6.5 above, but this time we fixed $\epsilon = t$ and considered a range of temperatures. From blue to red we have $k_b T = 0, \ 0.2t', \ 0.4t', \ t'$.

7 An Asymmetric 4-Site Ring

In this section we explore the results of our theory when applied to a ring of four sites (see fig.3.2), we consider again the wideband limit $t \gg t'$ and set $t = t''$. We choose the basis $\{|1\rangle, |2\rangle, |3\rangle, |4\rangle\}$ for the Hilbert space on the dot, where the numbering is as in fig.3.2. Hence we can write

$$H_d = \epsilon |2\rangle \langle 2| - t \left[|1\rangle \langle 2| + |1\rangle \langle 3| + |2\rangle \langle 4| + |3\rangle \langle 4| + \text{h.c.} \right] \qquad (7.0.1)$$

7.1 Computing the Green Function

Since our Hilbert space is now four-dimensional, inverting operators is no longer entirely trivial. Rather, we will need to invert a 4×4 matrix to find the Green function, $G^{R/A} = \left(\omega - H_d - \Sigma^{R/A} \right)^{-1}$, where one should note that ω is short-hand notation for the matrix $\omega \delta_{ij}$. We then have using (5.3.8) and (7.0.1)

$$\left(G^R \right)^{-1} = \begin{bmatrix} \omega & 0 & 0 & 0 \\ 0 & \omega & 0 & 0 \\ 0 & 0 & \omega & 0 \\ 0 & 0 & 0 & \omega \end{bmatrix} - \begin{bmatrix} 0 & -t & -t & 0 \\ -t & \epsilon & 0 & -t \\ -t & 0 & 0 & -t \\ 0 & -t & -t & 0 \end{bmatrix} - \Sigma \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} \omega - \Sigma & t & t & 0 \\ t & \omega - \epsilon & 0 & t \\ t & 0 & \omega & t \\ 0 & t & t & \omega - \Sigma \end{bmatrix},$$

where we have defined $\Sigma := -\frac{(t')^2}{t} e^{ik}$. Using either Cramer's[28] rule or a computer algebra programme the inverse is readily found to be $G^R = \hat{G}/\mathfrak{G}$ with

$$\hat{G} = \begin{bmatrix} \omega(\omega - \epsilon)(\omega - \Sigma) - \hat{G}_{41} & \hat{G}_{21} & \hat{G}_{31} & \hat{G}_{41} \\ -t\omega(\omega - \Sigma) & \omega(\omega - \Sigma)^2 - \hat{G}_{32} & \hat{G}_{32} & \hat{G}_{21} \\ -t(\omega - \epsilon)(\omega - \Sigma) & 2t^2(\omega - \Sigma) & (\omega - \epsilon)(\omega - \Sigma)^2 - \hat{G}_{32} & \hat{G}_{31} \\ t^2(2\omega - \epsilon) & \hat{G}_{21} & \hat{G}_{31} & \hat{G}_{11} \end{bmatrix},$$

and $\mathfrak{G} = \det\left(\left(G^R \right)^{-1} \right) = (\omega - \Sigma)\left(\omega(\omega - \epsilon)(\omega - \Sigma) - 2t^2(2\omega - \epsilon) \right)$.

From this way of presenting G^R it is clear that it possesses a lot of symmetries which can be related to symmetries of our model. The most obvious one is that the matrix $\hat{G}$ is symmetric, which is related to the fact that our system is invariant under time reversal. Another natural symmetry is that $\hat{G}_{ij} = \hat{G}_{\sigma(i)\sigma(j)}$ where σ is the map that exchanges 1 and 4, but fixes 2 and 3. This can be understood as a consequence of the reflection symmetry of our model, i.e. from the point of view of sites 2 and 3, the system looks identical to the left and right, nor is there an inherent difference between sites 1 and 4.

Additionally one can see a pattern in the the occurrence of powers of t. The elements $\hat{G}_{12}$ and $\hat{G}_{13}$ are linear in t, as they only represent a single hop. The elements $\hat{G}_{32}$

---

[28]Swiss, 1704-1752.

and $\hat{G}_{41}$ are quadratic in t, as they involve two hops (note that sites 2 and 3 are not directly connected, hence perhaps the factor 2 as there are two equivalent ways from 2 to 3). The diagonal terms are special, as they involve both terms without t and quadratic terms, however these quadratic terms always appear with a negative sign, so one could argue they represent transport away from the site. A peculiar phenomenon that one notices when one more closely examines the indices of these negative sign terms is that they always involve the site itself and the site farthest away (so 1-4 and 2-3 are paired).

Strikingly, the terms without t always seem to involve factors associated with all sites except the site in question (concretely $\omega - \epsilon$ is associated with site 2, $\omega = \omega - 0$ with 3, and $\omega - \Sigma$ with 1 and 4). This means that when the energy ω of the electron resonates with some other site this term vanishes and the only thing left is the outflow term. One could apply a similar analysis to the terms $\hat{G}_{12}$ and $\hat{G}_{13}$ to notice that for example $\hat{G}_{12}$ vanishes when the electron energy either resonates with site 1 or site 3.

Since we are interested in the element G_{41}^R to compute the transmission, we should mention the following somewhat difficult to interpret identity

$$G_{41}^R = \frac{G_{43}^R G_{21}^R}{G_{32}^R} + \frac{G_{42}^R G_{31}^R}{G_{23}^R} - G_{11}^R,$$

or equivalently

$$G_{11}^R = \frac{G_{12}^R G_{31}^R}{G_{23}^R} + \frac{G_{13}^R G_{21}^R}{G_{32}^R} - G_{14}^R.$$

The first identity can be viewed in light of the discussion above as extracting the outflow term from G_{11}^R using the other elements of the Green function to replicate the term without t. It seems that this needs to be done by taking some sort of mixed average of transport from 1 to 4 via 2 and 3 rather than for example via the more intuitive expression $G_{12}^R G_{24}^R$ (aside from the fact that this has the wrong units, another argument against its occurrence could be that it is indistinguishable from the expression $G_{12}^R G_{21}^R$ and hence cannot occur or cancels). It is interesting to note that the same equalities hold for the local Green function of the dot, which suggests that this effect is something that is inherent to the dot. Alternatively it is possible that this is simply a coincidental degeneracy due to the high symmetry of the model which allows only a few components of the Green function to behave independently.
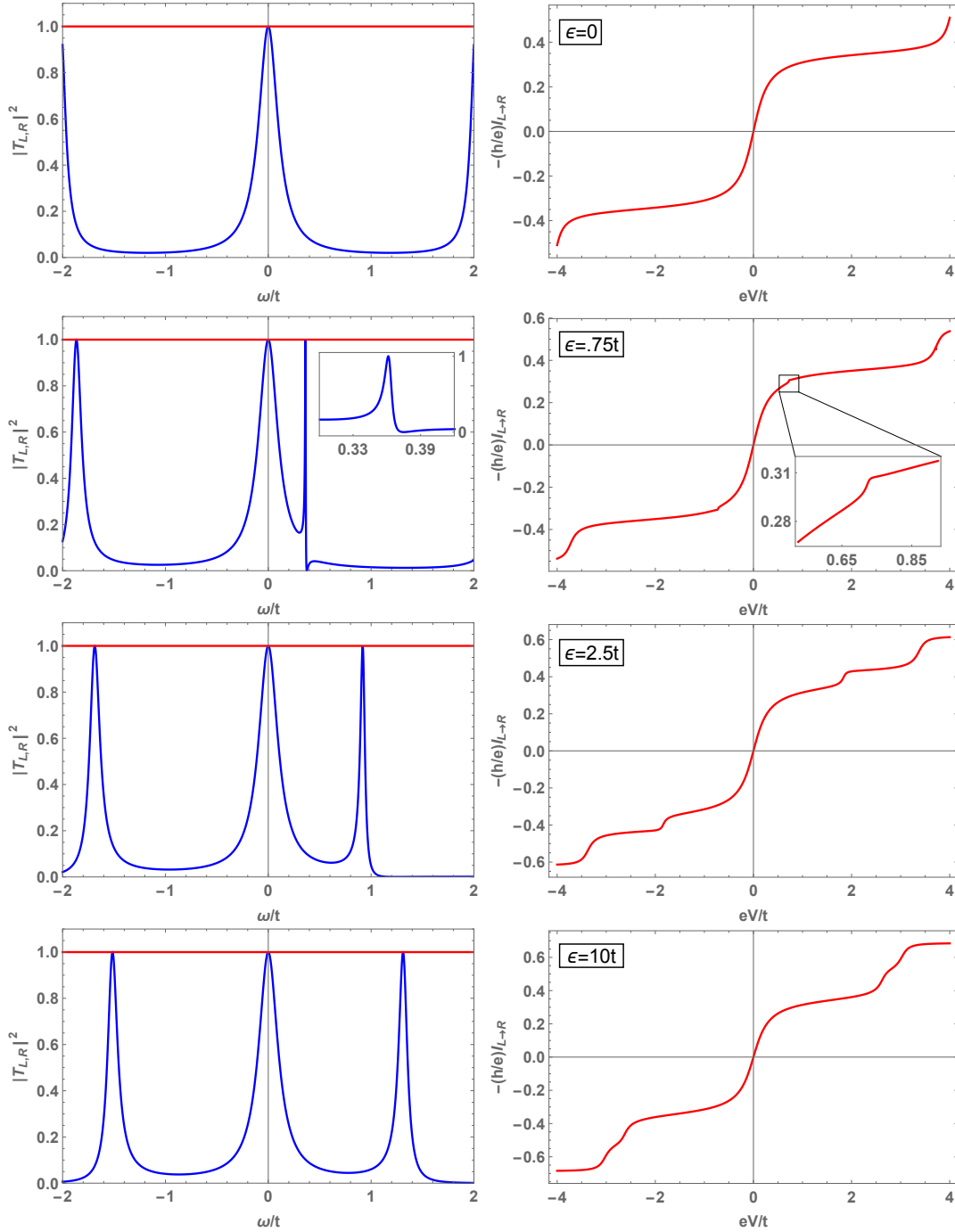
7.2 Behaviour of the Transmission

The relevant element of the Green function for transmission is as before

$$\langle 4 | G^R | 1 \rangle = \frac{t^2}{\omega - \Sigma} \frac{2\omega - \epsilon}{\omega(\omega - \epsilon)(\omega - \Sigma) - 2t^2(2\omega - \epsilon)},$$

and using the same formula as for the single site system we find

$$|T_{L,R}(\omega)|^2 = \Gamma_L(\omega)\Gamma_R(\omega)|\langle 4 | G^R(\omega) | 1 \rangle|^2,$$
$$= 2\pi t^4 \frac{\Gamma_L(\omega)\Gamma_R(\omega)}{\Gamma_{LR}(\omega)} \mathscr{L}_{\Gamma_{LR}(\omega)/2}(\omega - \mathfrak{Re}\,[\Sigma(\omega)])\mathscr{M}(\omega), \tag{7.2.1}$$

28

Figure 7.1: Left column: The transmission $(7.2.1)$ versus energy for the 4-site ring fig.3.2 with $t'' = t$, $t'/t = 1/3$ (this was chosen for numerical reasons, as the transmission was difficult to integrate for smaller values due to the narrowness of the peaks), and several values of ϵ; Clockwise: $\epsilon = 0, 0.75t, 10t, 2.5t$. **Right column:** A plot of the current versus bias computed from these transmission functions according to $(4.0.4)$ at 0 temperature; Clockwise: $\epsilon = 0, 0.75t, 10t, 2.5t$. The insets depict the same physical feature as seen in both the current and the transmission.
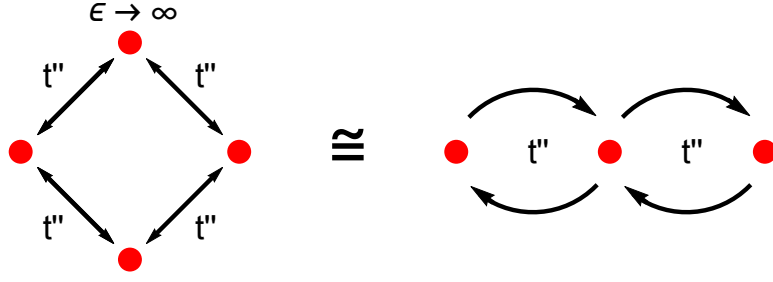
Figure 7.2: A cartoon of an equivalent characterisation of the nano-structure in the limit of infinite on-site energy. In this regime the top link is inaccessible and hence the system behaves like an isolated 3-chain with the same hopping (i.e. the lower link has been stretched into a straight line and the top site has been left out). For the transmission and current in this regime see fig.7.3.

where we have introduced

$$\Gamma_{L/R} := -\frac{(t')^2}{t}\sin(k), \ \Gamma_{LR} = \Gamma_L + \Gamma_R, \ \Sigma = \mathfrak{Re}\,[\Sigma] \mp \frac{i}{2}\Gamma_{LR},$$

in analogy with the single site system. Additionally $\mathscr{L}_\gamma(x_0)$ represents a Lorentzian distribution of width γ centred at x_0 and

$$\mathscr{M}(\omega) := \frac{(2\omega - \epsilon)^2}{(\omega(\omega - \epsilon)(\omega - \mathfrak{Re}\,[\Sigma]) - 2t^2(2\omega - \epsilon))^2 + (\omega(\omega - \epsilon)\Gamma_{LR}/2)^2}. \qquad (7.2.2)$$

The first few terms in (7.2.1) are very reminiscent of (6.0.2), but centred at $\omega - \mathfrak{Re}\,[\Sigma]$ instead of $\omega - \epsilon - \mathfrak{Re}\,[\Sigma]$. This can be understood as the contribution of the lower link of the system, where no barrier is present (looking at fig.7.1 one sees that this peak remains unchanged as ϵ varies). Additional features arise due to the modulating function $\mathscr{M}$, such as the other peaks and also strikingly a zero in the transmission, which upon inspection of (7.2.2) is seen to occur for $\omega = \epsilon/2$ (see the inset in the top right graph in fig.7.1).

Intuitively this zero makes some sense, since to an approaching electron with energy $\epsilon/2$ the system appears to be asymmetric, which one can expect to result in a phase difference between the upper and lower links of the ring. This is in fact what happens, recall that $\langle 4|G^R|1\rangle = \hat{G}_{41}/\mathfrak{G} = t^2(2\omega - \epsilon)/\mathfrak{G}$. One can interpret $\hat{G}_{41} \propto 2\omega - \epsilon$ as $\omega - 0 + \omega - \epsilon =: \Delta\omega_3 + \Delta\omega_2$, i.e. the propagation factor has two contributions, one from the lower link and one from the upper link. If $\omega = \epsilon/2$ we see that $\Delta\omega_2 = -\Delta\omega_3$ and thus their amplitudes are the same but the contributions are exactly out of phase and interfere destructively, hence this 0 is a self-interference effect.

The locations of the peaks in the transmission are easy to interpret, they correspond to energy levels of the system. If one takes the full wideband limit ($t' \to 0$), Σ vanishes and the peaks in the Green function should be located at the eigenvalues of H_d. One can do some analytical computations in the limiting cases $\epsilon = 0$ and $\epsilon \to \infty$ (for the next part we work in units of t). In the former case we can simply consider the Hamiltonian of an isolated chain of 4 sites with periodic boundary conditions,

$$H = \begin{bmatrix} 0 & -1 & -1 & 0 \\ -1 & 0 & 0 & -1 \\ -1 & 0 & 0 & -1 \\ 0 & -1 & -1 & 0 \end{bmatrix},$$
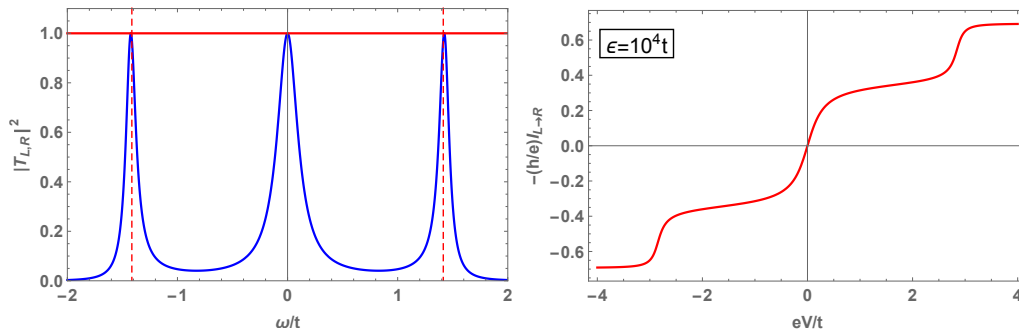
Figure 7.3: A plot of the transmission versus energy (left) and the current versus bias (right) for the limit case described in fig.7.2. The vertical dashed black lines are located at $\omega = \pm\sqrt{2}t$, the energy levels of this limit system. The slight deviation comes from the fact that our numerical computations are not in the true wideband limit.

which has eigenenergies $E = \pm 2, 0$, where 0 has multiplicity 2. Comparing to the case $\epsilon = 0$ in fig.7.1 (top left) we see that the two are in excellent agreement (up to a small shift due to our plots not being in the true wideband limit). For the latter case, the top link becomes inaccessible, and we can simply consider the Hamiltonian of a chain of length 3 (see fig.7.2),

$$H = \begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix},$$

with the resulting energies being $E = \pm\sqrt{2}, 0$. These results are summarized visually in fig.7.3 and fig.7.4.

However, fig.7.4 reveals more interesting information, namely that the slope of one of the eigenenergies that is shifted away from 0 with increasing ϵ is the same initially as the slope of the line that indicates the 0 in the transmission. This level corresponds for $\epsilon = 0$ to the eigenstate $\frac{1}{\sqrt{2}}(|2\rangle - |3\rangle)$, which intuitively does not contribute to the transmission directly. It also has exactly the asymmetry we discussed in the case of the zero so it makes sense that for small ϵ these phenomena behave similarly.

7.3 The Current

It is now a simple matter of integration according to (4.0.4) to obtain the current, the results can be seen in the lower half of fig.7.1.

As one would expect from the above discussion, the overall profile of the current is dominated by the central peak in the transmission, and the smaller features can readily be linked to the previous section. In the limit of large ϵ (bottom right in fig.7.1 or on the left in fig.7.3) we see that the only features left are the three levels we discussed earlier. It is however interesting to note that a stronger barrier amplifies the current instead of diminishing it as we saw for the single impurity. One can see this in fig.7.5, where the maximal current as a function of the on-site energy is plotted. This is due to the fact that the energy levels for the 3-chain are fully contained in the band, whereas the non-zero energy levels for the 4-chain are right on the edge. In light of the zero in the transmission one could argue that additionally for finite
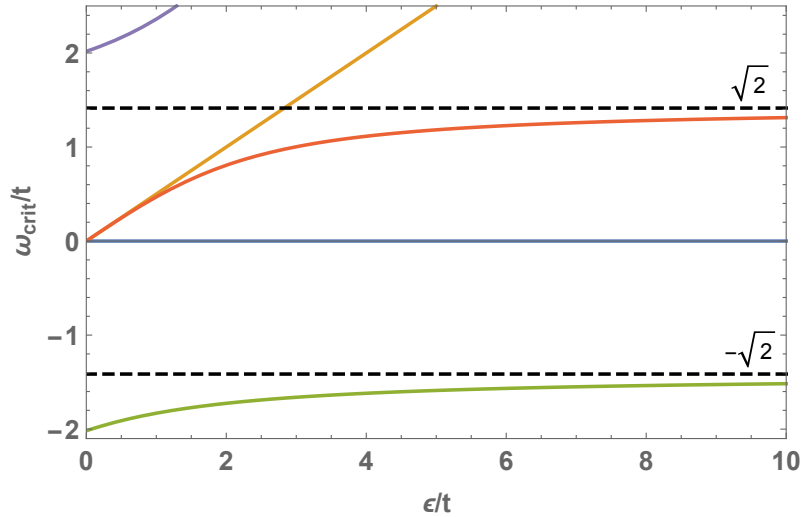
Figure 7.4: A plot of the extremising values of ω for the transmission (7.2.1) and the eigenenergies of H_d (visually indistinguishable) as a function of ϵ.

barrier strengths the current does not reach its maximum due to interference effects between the two links (note also that for $\epsilon/t \approx 4$ when the zero leaves the band, the current does not grow much more).

Finally we consider the non-zero temperature case, plotted in fig.7.6. As expected, nothing surprising happens and the interpretation is the same as for the single site system (mutatis mutandis).
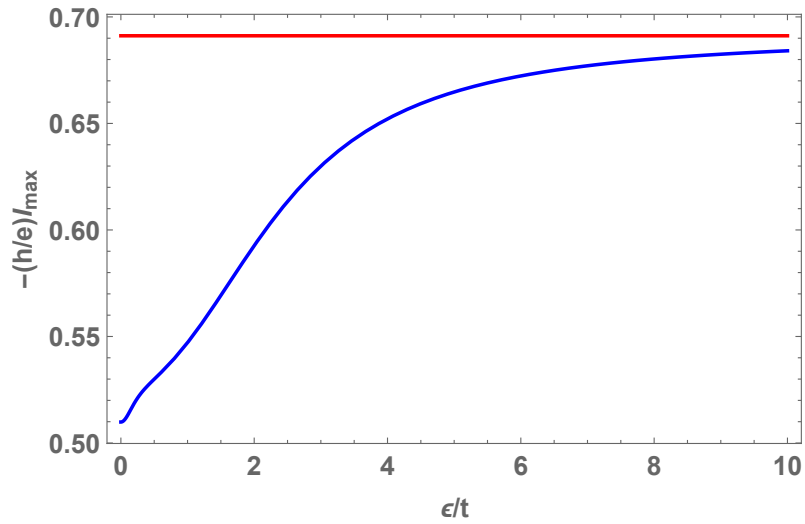
Figure 7.5: The maximal current (i.e. the transmission integrated over the full bandwidth) as a function of ϵ. The red line marks the limiting value as ϵ grows to infinity.
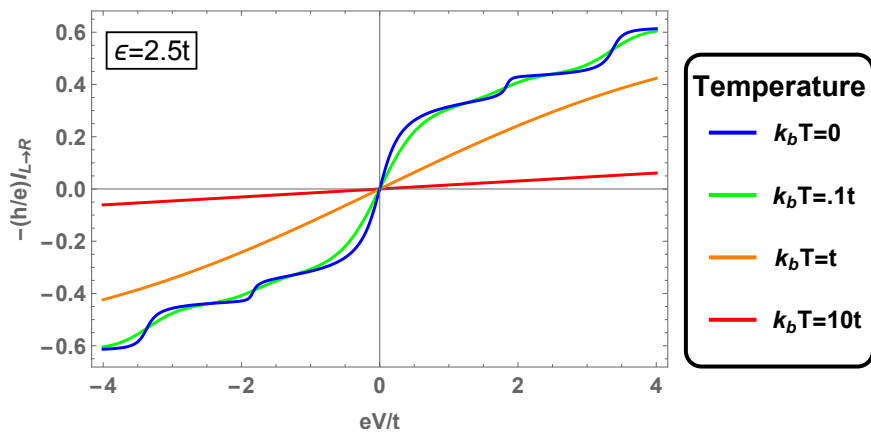
Figure 7.6: The current from fig.7.1, but this time we fixed $\epsilon = 2.5t$ and considered a range of temperatures. From blue to red we have $k_bT = 0, 0.1t, t, 10t$.

8 Outlook

In this section we discuss (semi-heuristically) some possible generalisations of the model and the challenges they present. At the same time this section can be seen as a limited overview of recent and current research in the field of mesoscopic transport physics.

One might have noted that in our discussion so far, we have been able to avoid using any non-equilibrium or many-body techniques, even though we were dealing with a transport problem on a mesoscopic scale. In a sense we have been very fortunate, because we shall see that this will no longer work for more sophisticated models.

8.1 Interactions and the Meir-Wingreen Formula

Including nearest neighbour interactions within the dot sounds innocent enough, but this additional term causes our single-particle, elastic scattering approach to break down completely. This means that we cannot use (4.0.4) to calculate the current, even if we had the full "interacting single particle Green function"[29]. We now need to consider many-particle processes, which entail keeping track of several particles at once, even for the single-particle Green function. Additionally the interactions induce non-trivial correlations between particles that extend into the leads. Consider for example the case of the 4-ring where a particle is present at say site 2, then a particle that wants to tunnel from the left reservoir into the dot (site 1) is penalised for doing so by the nearest-neighbour interaction. Fortunately, there does exist a suitable generalisation of the Landauer-Büttiker formalism.

In 1992, Yigal Meir[30] and Ned Wingreen[31] published [14], a paper in which they proposed (in their own words) a *Landauer formula* for the current through an interacting region. Note that this paper was published 45(!) years after Landauer's own work [11]. Their formula in its full generality (eq.(6) in [14]) cannot be meaningfully stated here, as it makes use of the machinery of the Keldysh formalism, which is far beyond the scope of this thesis. However, if one assumes that the coupling of the nano-structure to the leads is *proportional* in the sense that $\Gamma_L(\omega) = \lambda \Gamma_R(\omega)$ for some scalar λ, a suitable superposition of the leads can be chosen in such a way that the current formula simplifies to

$$I_\alpha = -\frac{2e}{h} \int dE \left[f_L(E) - f_R(E) \right] \mathfrak{Im} \left\{ \mathrm{tr}\big(\Gamma_{LR} G^R \big) \right\}, \qquad (8.1.1)$$

where $\Gamma_{LR} = \Gamma_L \Gamma_R / (\Gamma_L + \Gamma_R)$ (eq.(9) in [14], compare with (6.0.2)).

The imaginary part of the Green function is usually called the *spectral function* and loosely speaking it encodes how well excitations in the system can be described as free particles (one can show that for diagonal/quadratic Hamiltonians this is always a delta function), the product with Γ_{LR} suggests some additional broadening of this function due to the coupling. Heuristically speaking one can read the above formula

---

[29]We will not give precise definitions in this section, as it requires theory beyond the scope of this thesis.

[30]Israeli, 19??-.

[31]American, 19??-.

as saying that per energy E one needs to measure availability in the reservoirs and multiply by a factor that described how free-particle-like this excitation will be, i.e. to what extend it propagates like the scattered states we have been considering in this thesis. It is important to note that the proportionally assumption does NOT hold for the 4-ring from chapter 7. The Γ's are operators, and in the case of the 4-ring not all sites in the dot are coupled to the (same) leads, violating the proportionally assumption. It would however be valid for the single impurity from chapter 6.

A class of models called *Anderson-type models* usually do satisfy this requirement. They were introduced by Paul Anderson in his 1961 paper [2] (compare section II of this paper to chapter 3 of this thesis). Instead of there being "spatial" levels like in our case, the model considers a single site that has one or several energy levels[32], all of which are coupled to the reservoirs[33]. Additionally these models differ from what we treat here in that they almost always include spin-effects. For this family of Hamiltonians, the above current formula (8.1.1) is very useful.

If one defines the interacting self energy according to $\Sigma^{R/A} = (g^{R/A})^{-1} - (G^{R/A})^{-1}$ (compare with (5.3.4)), one can write $G^R - G^A = G^R \Sigma G^A$ with $\Sigma = \Sigma^R - \Sigma^A$. Using this and (5.3.6) we can rewrite (8.1.1) as

$$
\begin{aligned}
I_\alpha &= \frac{ie}{h} \int \mathrm{d}E \left[f_L(E) - f_R(E) \right] \mathrm{tr} \left\{ \Gamma_{LR} (G^R - G^A) \right\}, \\
&= \frac{ie}{h} \int \mathrm{d}E \left[f_L(E) - f_R(E) \right] \mathrm{tr} \left\{ \frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R} G^R \Sigma G^A \right\}, \\
&= \frac{e}{h} \int \mathrm{d}E \left[f_L(E) - f_R(E) \right] \mathrm{tr} \left\{ G^A \Gamma_R G^R \Gamma_L \left(-i\Gamma_L - i\Gamma_R \right)^{-1} \Sigma \right\}, \\
&= \frac{e}{h} \int \mathrm{d}E \left[f_L(E) - f_R(E) \right] \mathrm{tr} \left\{ G^A \Gamma_R G^R \Gamma_L \Sigma_0^{-1} \Sigma \right\},
\end{aligned}
$$

where Σ_0 is the non-interacting self-energy. Note the similarities with (5.3.10), and it even seems plausible that in the non-interacting limit the two coincide (provided the limit is not singular).

8.2   AC-Conductance

Another possible, more modest generalisation would be to consider what happens if the system is driven by AC instead of the more battery-like constant chemical potential difference we have considered so far. The quantity of interest in such situations is often the AC conductance $G(\omega)$. A difficulty that immediately becomes apparent is that this is not an equilibrium quantity, and non-equilibrium techniques are beyond the scope of this thesis.

Fortunately, it is possible to compute the linear response AC conductance (we shall make no notational distinction) using only equilibrium objects. This is due to the so called *Kubo formula*, which we shall derive in the next section. We will then heuristically show how one can write down expressions for the relevant observables and attempt to apply them to our system. Recall that we in fact already have a

---

[32]The canonical Anderson model has a single level, see also [1] which treats a slightly more general model.

[33]Of course one can construct models where this symmetry is broken, but those are unusual.

prediction for the DC limit of this quantity, see (4.0.6). In the last section we will show that this prediction is recovered if one considers $\lim_{\omega \downarrow 0} G(\omega)$. For details one may consult chapters 6 and section 7.2.2 of [4].

8.2.1 Linear Response Theory

We wish to investigate the dynamics of the Hamiltonian

$$H = H_0 + V(t),$$

where we assume that we have solved the time independent problem H_0 and we view V as a small perturbation. To this end we introduce the so called *interaction picture* state vectors and operators,

$$\left| \hat{\psi}(t) \right\rangle := e^{\frac{i}{\hbar} H_0 t} \left| \psi(t) \right\rangle, \ \hat{O} := e^{\frac{i}{\hbar} H_0 t} O e^{-\frac{i}{\hbar} H_0 t}.$$

The main idea behind these definitions is to extract the "trivial" evolution due to H_0. The governing equation in this picture is given by

$$i\hbar \partial_t \left| \hat{\psi}(t) \right\rangle = \left(i\hbar \partial_t e^{\frac{i}{\hbar} H_0 t} \right) \left| \hat{\psi}(t) \right\rangle + e^{\frac{i}{\hbar} H_0 t} \left(i\hbar \partial_t \left| \psi(t) \right\rangle \right) = \hat{V}(t) \left| \hat{\psi}(t) \right\rangle.$$

This suggests the existence of a unitary operator that evolves a state from say time t_0 to t, i.e.

$$\left| \hat{\psi}(t) \right\rangle = \hat{U}(t, t_0) \left| \hat{\psi}(t_0) \right\rangle,$$

and hence we must have $\hat{U}(t_0, t_0) = 1$. Substituting this into the governing equation we find that $\hat{U}$ is determined by the recursive integral equation

$$\hat{U}(t, t_0) = 1 + \frac{\hbar}{i} \int_{t_0}^{t} \mathrm{d}s \ \hat{V}(s) \hat{U}(s, t_0).$$

If the perturbation is small or if we are content with linear response, we can say to first order in $\hat{V}$ that

$$\hat{U}(t, t_0) \simeq 1 - i\hbar \int_{t_0}^{t} \mathrm{d}s \ \hat{V}(s). \tag{8.2.1}$$

Suppose now that $V(t) = \vartheta(t - t_0) H'$, i.e. the perturbation is switched on at some time t_0. What happens to the ensemble average of an operator at times later than t_0? Recall from statistical mechanics that

$$\langle O(t) \rangle = \frac{1}{Z_0} \sum_n \langle n(t) | O | n(t) \rangle \, e^{-\beta E_n},$$

where Z_0 is the partition function in equilibrium. We assume that the perturbation does not change the energies, the states, or the form of the operator O, but only their evolution (hence we use Z_0). In light of our discussion above this can be rewritten as

$$\langle O(t) \rangle = \frac{1}{Z_0} \sum_n \langle \hat{n}(t_0) | \hat{U}^\dagger(t, t_0) \hat{O}(t) \hat{U}(t, t_0) | \hat{n}(t_0) \rangle,$$

but by definition $|\hat{n}(t_0)\rangle = |n\rangle$. We now use (8.2.1) and collect the terms up to linear order to find

$$\langle O(t) \rangle \simeq \langle O \rangle_0 - i\hbar \int_{t_0}^{t} \mathrm{d}s \ \vartheta(s - t_0) \left\langle \left[\hat{O}(t), \hat{H}'(s) \right] \right\rangle_0, \tag{8.2.2}$$

where $\langle \ldots \rangle_0$ denotes an equilibrium average. This is the celebrated Kubo formula, which was first derived in [10] by Ryogo Kubo[34]. The power of this result lies in the fact that a deviation from equilibrium can be computed solely using equilibrium wavefunctions and statistics.

If the perturbing operator has the form $H'(t) = Af(t)$, where f is simply a function, the result simplifies considerably in frequency space. To see this we first introduce the so called *retarded correlation function*,

$$\langle O(t) \rangle - \langle O \rangle_0 =: \delta \langle O(t) \rangle =: \int_{t_0}^{\infty} \mathrm{d}s \ C_{O,H'}^{R}(t, s).$$

If we are not interested in transient behaviour, we can send $t_0 \to -\infty$. C^R should then only be a function of the time difference and we have

$$\delta \langle O(t) \rangle = \int_{-\infty}^{\infty} \mathrm{d}s \ C_{O,A}^{R}(t - s)f(s) = \left(C_{O,A}^{R} * f \right)(t),$$

which is convolution. Since $\mathcal{F}(g * h) = \mathcal{F}(g)\mathcal{F}(h)$ we find in the frequency domain that

$$\delta \langle O(\omega) \rangle = C_{O,A}^{R}(\omega)f(\omega). \tag{8.2.3}$$

8.2.2 Conductivity and Conductance from the Kubo Formula

We now present a sketch of the derivation of the conductivity and conductance in linear response. Consider a systems of electrons that are perturbed by a spatially uniform, but time dependent external electromagnetic field. If we make the gauge choice $\varphi_{\mathrm{ext}} = 0$ we have simply that $\mathbf{E}_{\mathrm{ext}}(t) = -\partial_t \mathbf{A}_{\mathrm{ext}}(t)$, or $\mathbf{A}_{\mathrm{ext}}(\omega) = (1/i\omega)\mathbf{E}_{\mathrm{ext}}(\omega)$. Recall that the conductivity tensor σ is defined by the relation

$$\mathbf{I}_e(\mathbf{r}, \omega) = \int \mathrm{d}\mathbf{r}' \ \sigma(\mathbf{r}, \mathbf{r}', \omega)\mathbf{E}(\omega),$$

and the linear conductance G as

$$\mathbf{I}_e(\omega) = G(\omega)V.$$

This definition agrees with (4.0.6) since we work in linear order of V in this section. Note that $\mathbf{I}_e(\mathbf{r}, \omega)$ is the current density, whereas $\mathbf{I}_e(\omega)$ is the total current.

To see how the electrons couple to the field in linear order, we take a look at the classical case. One can show that upon applying the Euler-Lagrange equations, the following Lagrangian yields the correct equations of motion,

$$\mathscr{L} = \frac{1}{2}m\dot{\mathbf{x}}^2 - q\varphi + q\dot{\mathbf{x}} \cdot \mathbf{A}.$$

---

[34] Japanese, 1920-1995.

The conjugate coordinate is then the so called *kinematic momentum* $\mathbf{p} = m\dot{\mathbf{x}} + q\mathbf{A}$, which results in the Hamiltonian

$$\mathscr{H} = \frac{1}{2m}\left(\mathbf{p} - q\mathbf{A}\right)^2 + q\varphi.$$

Taking the functional derivative with respect to $\mathbf{A}$ yields

$$\delta\mathscr{H} = -q\dot{\mathbf{x}} \cdot \delta\mathbf{A} = -\int d\mathbf{r} \ (q\mathbf{J}) \cdot \mathbf{A},$$

and hence

$$H'(t) = e\mathbf{A}_{\text{ext}}(t) \cdot \int d\mathbf{r} \ \mathbf{J}(\mathbf{r}).$$

However, the particle current density operator $\mathbf{J}$ is not exactly the same as in (2.1.3) due to the presence of the field (due to its explicit appearance above in $\mathscr{H}$). One can show that in this case $\mathbf{J} = \mathbf{J}^{\nabla} + \frac{e}{m}\mathbf{A}\rho(\mathbf{r})$, where $\mathbf{J}^{\nabla}$ is the usual particle current density operator and $\rho(\mathbf{r})$ the electron density. These contributions are called the paramagnetic and diamagnetic term respectively (note that the second term is proportional to $-q$). Nevertheless, we may disregard this second contribution in H', as it generates a higher order correction, thus

$$H'(\omega) = \frac{e}{i\omega}\mathbf{E}(\omega) \cdot \int d\mathbf{r} \ \mathbf{J}^{\nabla}(\mathbf{r}). \tag{8.2.4}$$

Since $\mathbf{I}_e(\mathbf{r}, \omega) = -e\langle \mathbf{J}(\mathbf{r}, \omega)\rangle$, we compute the right hand side and compare with the definitions of the quantities above.

$$\langle \mathbf{J}(\mathbf{r}, \omega)\rangle = \langle \mathbf{J}^{\nabla}(\mathbf{r})\rangle(\omega) + \left\langle \frac{e}{i\omega m}\mathbf{E}(\omega)\rho(\mathbf{r})\right\rangle \simeq \langle \mathbf{J}^{\nabla}(\mathbf{r})\rangle(\omega) + \frac{e}{i\omega m}\mathbf{E}(\omega)\langle\rho(\mathbf{r})\rangle_0,$$

as incorporating effects of the fields on the electron density gives higher order terms that we do not consider here. It remains to tackle to first term, for this we use what we derived in the last section, specifically (8.2.3). We may use this form since (8.2.4) is obviously of the form $Af(\omega)$. Additionally we only need to keep this deviation from equilibrium, as our equilibrium state carries no net current. Putting all of this together we arrive at

$$\langle \mathbf{J}(\mathbf{r}, \omega)\rangle \simeq \left[\int d\mathbf{r}' \frac{e}{i\omega}C^R_{\mathbf{J}^{\nabla}(\mathbf{r})\mathbf{J}^{\nabla}(\mathbf{r}')}(\omega) + \frac{e}{i\omega m}\langle\rho(\mathbf{r})\rangle_0\right]\mathbf{E}(\omega),$$

from which we can read off that

$$\sigma^{\alpha\beta}(\mathbf{r}\,\mathbf{r}', \omega) = \frac{e^2\langle\rho(\mathbf{r})\rangle_0}{mi\omega}\delta(\mathbf{r} - \mathbf{r}')\delta_{\alpha\beta} - \frac{e^2}{i\omega}\Xi_{\alpha\beta}(\mathbf{r}, \mathbf{r}', \omega), \tag{8.2.5}$$

where Ξ is the retarded correlation tensor in frequency space between the α and β components of the particle current density operator evaluated at $\mathbf{r}$ and $\mathbf{r}'$ respectively.

To find the conductance we need to integrate the above current density over some cross-section. Since field lines of electromagnetic fields away from sources are submanifolds, we can pick an equipotential plane as this cross-section on which we have

coordinates $\mathbf{y}_z$ and a perpendicular coordinate z. This is helpful as in these coordinates $\mathbf{E}(\omega) = E(\omega)\hat{z}$. Performing this integral amounts to

$$\mathbf{I}_e(z, \omega) = \int \mathrm{d}\mathbf{y}_z \hat{z} \cdot \mathbf{I}_e(z, \mathbf{y}_z, \omega) = \int \mathrm{d}\mathbf{y}_z \int \mathrm{d}\mathbf{r}' \hat{z} \cdot \left[\sigma((\mathbf{y}_z, z), \mathbf{r}', \omega)E(\omega)\hat{z}'\right],$$

$$= \int \mathrm{d}\mathbf{y}_z \int \mathrm{d}\mathbf{y}_z' \int \mathrm{d}z' \hat{z} \cdot \left[\sigma((\mathbf{y}_z, z), (\mathbf{y}_z', z'), \omega)E(\omega)\hat{z}'\right].$$

We are only interested in the real part of the current, and noting that $\int \mathrm{d}\mathbf{y}_z \hat{z} \cdot \mathbf{J} =: \mathbf{I}(z)$ is the total particle current at cross-section z we can reduce this to

$$\mathbf{I}_e(z, \omega) = \int \mathrm{d}z' \, \mathfrak{Re}\left[\frac{ie^2}{\omega} C^R_{\mathbf{I}(z)\mathbf{I}(z')}\right] E(\omega).$$

However, due to current conservation, there should be no dependence on z. It is good to recall here that we are interested in the conductance measured across the reservoirs, so we are always far away from the nano-structure, where this argument holds undoubtedly. By similar reasoning one can show that in fact there is also no dependence on z' in the current-current correlator and then the integration over z' simply gives rise to the voltage difference ($\int \mathrm{d}z' E = V$) and we find

$$G(\omega) = -\mathfrak{Im}\left[\frac{e^2}{\omega} C^R_{\mathbf{II}}(\omega)\right]. \tag{8.2.6}$$

In the context of our system we can write

$$H' = \frac{eV}{2}\cos(\omega t)(N_L - N_R),$$

where N_α is the operator that counts the number of particles in reservoir α. Note that it is related to the particle current by the relation $\langle \mathbf{I}_\alpha \rangle = \langle \dot{N}_\alpha \rangle$, and in steady state we have $\langle \mathbf{I}_L \rangle = -\langle \mathbf{I}_R \rangle = (\langle \mathbf{I}_L \rangle - \langle \mathbf{I}_R \rangle)/2$. From elementary quantum mechanics we know that the time derivative of an operator is equal to its commutator with the Hamiltonian, hence $\dot{N}_\alpha = i[H, N_\alpha]$. Therefore the quantity we need to compute is the Fourier transform of

$$C^R_{\mathbf{I}(t), \mathbf{I}(0)} \propto i\theta(t)\left\langle [\dot{N}_L(t) - \dot{N}_R(t), \dot{N}_L(0) - \dot{N}_R(0)]\right\rangle_0.$$

The first step is to determine $[H, N_\alpha] = [H_t, N_\alpha]$ (because that is the only part of the Hamiltonian that does not conserve the number of particles in reservoir α), which we do in k-space where N_α is diagonal and there are coefficients t_k such that

$$[H_t, N_\alpha] = \sum_{k,k'}\left[t_k d_\alpha c_k^\dagger + t_k^* d_\alpha^\dagger c_k, N_{k'}\right],$$

$$= \sum_{k,k'}\left\{t_k d_\alpha[c_k, N_{k'}] + t_k^* d_\alpha^\dagger[c_k^\dagger, N_{k'}]\right\},$$

$$= \sum_k \left\{t_k d_\alpha[c_k, N_k] + t_k^* d_\alpha^\dagger[c_k^\dagger, N_k]\right\},$$

$$= \sum_k \left\{-t_k d_\alpha c_k^\dagger + t_k^* d_\alpha^\dagger c_k\right\} = t' c_0^\dagger d_\alpha - \text{h.c.}.$$

This result is rather intuitive, since the first term in the final result adds a particle to the reservoir and hence gives a positive contribution to $\dot{N}_\alpha$ (the second terms is interpreted in the same way).

However, this poses a problem. The operator whose correlator we need to calculate connects the subspaces of our Hilbert space and hence we need the full wavefunctions to evaluate the expectation values involved in the ensemble average. Despite having solved the DC problem, we do not have these wavefunctions, as we only considered scattering Ansätze and these say nothing about what happens inside the nano-structure. One would in all likelihood not see this in linear response, but in principle the internal processes of the nano-structure can be non-trivial and take a long time to decay (see chapter 4 of [16], for example fig 4.15.).

8.2.3 Relation to Landauer-Büttiker

Even though we are not able to compute $G(\omega)$ with the methods provided in this thesis, we can still show that if one makes similar assumptions as in our derivation of (4.0.4) (i.e. using scattering states and taking the DC limit), the two formulae agree. If we expand (8.2.6) we find

$$G(\omega) = -\frac{e^2}{\omega}\mathfrak{Im}\left[\int_{-\infty}^{\infty} dt\ e^{i(\omega+i\eta)t}(-i)\theta(t)\left\langle[I(t),I(0)]\right\rangle_0\right], \qquad (8.2.7)$$

where $\eta = 0^+$ is a convergence factor. We begin by evaluating the commutator. To this end we expand the current operator I in the scattering basis $\lambda = (\alpha, E)$ (see (2.5.1)), this yields

$$I = \sum_{\lambda,\lambda'} j_{\lambda\lambda'}^x c_\lambda^\dagger c_{\lambda'},$$

where the matrix element[35]

$$j_{\lambda\lambda'}^x = \frac{1}{2mi}\int d\mathbf{r}\ \psi_\lambda^*\left(\overrightarrow{\partial}_x - \overleftarrow{\partial}_x\right)\psi_{\lambda'},$$

carries the superscript x to remind us that it was calculated in the position representation (this will become important later). The time dependence comes into the current operator via the creation and annihilation operators, but since we work in the scattering basis their time dependence is trivial and we can write

$$\left\langle[I(t),I(0)]\right\rangle_0 = \sum_{\lambda,\lambda',\nu,\nu'} j_{\lambda\lambda'}^x j_{\nu\nu'}^x\ e^{i(E_\lambda - E_{\lambda'})t}\left\langle[c_\lambda^\dagger c_{\lambda'}, c_\nu^\dagger c_{\nu'}]\right\rangle_0.$$

Using the commutator identity (2.4.4) we find

$$[c_\lambda^\dagger c_{\lambda'}, c_\nu^\dagger c_{\nu'}] = c_\lambda^\dagger[c_{\lambda'}, c_\nu^\dagger]c_{\nu'} + [c_\lambda^\dagger, c_\nu^\dagger]c_{\lambda'}c_{\nu'} + c_\nu^\dagger c_\lambda^\dagger[c_{\lambda'}, c_{\nu'}] + c_\nu^\dagger[c_\lambda^\dagger, c_{\nu'}]c_{\lambda'}.$$

From (2.4.3) one easily deduces that

$$[c_a^\dagger, c_b^\dagger] = 2c_a^\dagger c_b^\dagger,\ \ [c_a, c_b] = 2c_a c_b,\ \ [c_a^\dagger, c_b] = 2c_a^\dagger c_b - \delta_{ab},$$

---

[35]The arrows indicate on which side the derivative acts.

and hence after some manipulations

$$[c_\lambda^\dagger c_{\lambda'}, c_\nu^\dagger c_{\nu'}] = \delta_{\lambda'\nu} c_\lambda^\dagger c_{\nu'} - \delta_{\lambda\nu'} c_\nu^\dagger c_{\lambda'}.$$

Consider the quantity $\langle c_a^\dagger c_b \rangle_0$, if $a \neq b$ it should vanish, as there is no movement in equilibrium. This leaves the case $a = b$, then we are computing the equilibrium average of the number operator, which is simply the fermi-dirac distribution f evaluated at the relevant energy. Thus $\langle c_a^\dagger c_b \rangle_0 = \delta_{ab} f(E_a)$ and

$$\left\langle [c_\lambda^\dagger c_{\lambda'}, c_\nu^\dagger c_{\nu'}] \right\rangle_0 = \delta_{\lambda'\nu} \delta_{\lambda\nu'} \left[f(E_\lambda) - f(E_{\lambda'}) \right].$$

With the additional remark that $j_{ab}^x = (j_{ba}^x)^*$ we have simplified (8.2.7) to

$$G(\omega) = -\frac{e^2}{\omega} \sum_{\lambda,\lambda'} |j_{\lambda\lambda'}^x|^2 \left[f(E_\lambda) - f(E_{\lambda'}) \right] \mathfrak{Im} \left[\int_0^\infty dt (-i) e^{i(\omega + i\eta + E_\lambda - E_{\lambda'})t} \right].$$

It is easy to see that the integral evaluates to

$$\mathfrak{Im} \left[\int_0^\infty dt (-i) e^{i(\omega + i\eta + E_\lambda - E_{\lambda'})t} \right] = \mathfrak{Im} \left[\frac{1}{\omega + i\eta + E_\lambda - E_{\lambda'}} \right],$$
$$= -\frac{\eta}{\eta^2 + (\omega + E_\lambda - E_{\lambda'})^2},$$

which becomes $-\pi \delta(\omega + E_\lambda - E_{\lambda'})$ for $\eta \downarrow 0$. If we now take the DC limit

$$\lim_{\omega \downarrow 0} G(\omega) = \lim_{\omega \downarrow 0} e^2 \pi \sum_{\lambda,\lambda'} |j_{\lambda\lambda'}^x|^2 \frac{f(E_\lambda) - f(E_{\lambda'})}{\omega} \delta(\omega + E_\lambda - E_{\lambda'}),$$

we see that the fraction converges to a derivative due to the delta function and the DC limit, in symbols

$$G(0) = e^2 \pi \sum_{\lambda,\lambda'} |j_{\lambda\lambda'}^x|^2 \left(-\frac{\partial f(E_\lambda)}{\partial E_\lambda} \right) \delta(E_\lambda - E_{\lambda'}),$$

and therefore in the limit of zero temperature,

$$G(0) = e^2 \pi \sum_{\lambda,\lambda'} |j_{\lambda\lambda'}^x|^2 \delta(E_\lambda - \mu) \delta(E_\lambda - E_{\lambda'}).$$

Recalling that $\lambda = (\alpha, E)$, we can replace $\sum_\lambda \rightarrow \sum_\alpha \frac{m}{2\pi} \int dE$ to find

$$G(0) = e^2 \pi \frac{m^2}{4\pi^2} 2 \left| j_{(L,\mu)(R,\mu)}^x \right|^2,$$

which already looks very similar to (4.0.6). When we compare the definitions of j and T from our computation of the current operator elements in chapter 4, we see that there is a factor $\hbar$ difference due to unit convention, and another factor $(2\pi/m)^2$ as we computed T via energy and j in space. Putting this together we find the desired equality

$$\lim_{\omega \downarrow 0} G(\omega)^{\text{scatt.states}} = \frac{e^2}{h} |T_{L,R}(\mu)|^2.$$

41

8.3 Transient Behaviour

All of our investigations thus far, even the two more sophisticated cases above, have focused on obtaining steady-state quantities of the system. As mentioned in the previous section, cases where transient behaviour is non-trivial are known. For applications in electronics, knowledge of start-up effects and response to changes in voltage, etc. is important. To this end one would have to quench the system at some time t_0 and study the resulting time dependent dynamics.

There exists an extension to the Landauer-Büttiker formula that aims to give a fully dynamical description. It was introduced in 2014 with the paper [18], but the author is not aware of any work based on this description other than that given in the paper.

Another pen and paper approach is to use perturbation theory in the form of the *quantum master equation* (see [7]). In this approach one writes down differential equations that govern the time-evolution of the *density operator* ρ[36] which has the property that $\langle O \rangle = \text{Tr}[\rho O]$. The structure of these equations is (in certain approximations/limits) comparable to the Kolmogorov equations from stochastic processes theory. The method is perturbative in the sense that one needs to calculate contributions in orders of the dot-reservoir coupling when the usual von Neumann equation of motion $i\hbar\partial_t\rho = [H, \rho]$ is approximated by $[H_{\text{dot}}, \rho_{\text{dot}}]$ on the RHS. Usually (e.g. for the Anderson model and most other simple cases) this zero-eth order term is purely real and will only cause unitary oscillations. In analogy with the self-energy we have seen arise in chapter 5, the higher order contributions will include finite imaginary terms that induce actual transitions.

Alternatively one could turn to numerics, as in [16].

All avenues are areas of ongoing research and any attempt to treat them is beyond the scope of this thesis.

---

[36]Note that often this approach does not consider the full density operator, but rather the restriction to the nano-structure (via tracing out the reservoirs), which is commonly projected onto n-particle state manifolds.

Appendix A   The Reservoir Integral

In this section we will derive the result

$$\left\langle n, \beta \left| \frac{1}{\epsilon_k - H_{\mathrm{res}}^{\beta} + i\eta} \right| 1, \beta \right\rangle = -\frac{e^{ikn}}{t},$$

which was used in section 5 (see (5.1.4)). The first step is to use the basis of plane waves for the chain (which is also an eigenbasis for the sandwiched operator) to write

$$\left\langle n, \beta \left| \frac{1}{\epsilon_k - H_{\mathrm{res}}^{\beta} + i\eta} \right| 1, \beta \right\rangle = \int_0^{\pi} \left\langle n, \beta \middle| \psi_{\beta,k'}^{(0)} \right\rangle \frac{1}{\epsilon_k - \epsilon_{k'} + i\eta} \left\langle \psi_{\beta,k'}^{(0)} \middle| 1, \beta \right\rangle \mathrm{d}k',$$

$$= \int_0^{\pi} \frac{2}{\pi} \sin(nk') \sin(k') \frac{1}{-2t(\cos(k) - \cos(k')) + i\eta} \mathrm{d}k',$$

$$= \frac{1}{\pi} \int_{-\pi}^{\pi} \frac{\sin(nk') \sin(k')}{-2t(\cos(k) - \cos(k')) + i\eta} \mathrm{d}k'.$$

To evaluate this integral, we make the substitution $z = e^{ik'}$ and use the complex
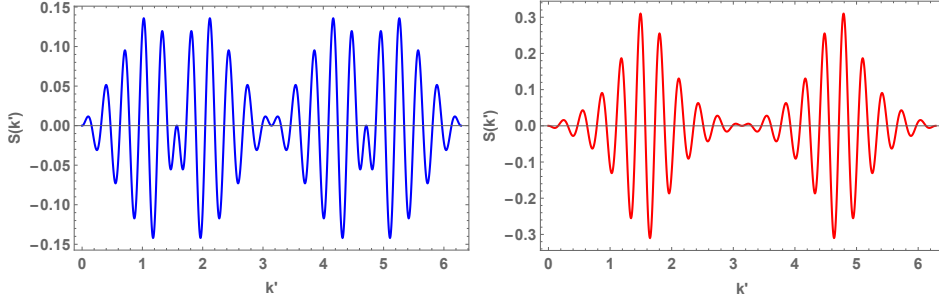
Figure A.1: A plot of the real (blue) and imaginary (red) part of the integrand above. The parameters were set to $n = 20$, $k = \pi/2$, $t = 1$, $\eta = 1$.

exponential form for the trigonometric functions. This transforms the problem into a contour integral along the unit circle in the complex plane, which we will evaluate using the Residue Theorem, a useful consequence of Cauchy's integral formula. An excellent reference for the complex analysis required for this section is [12], in particular chapter VI §1 (Theorem 1.2). In symbols we have
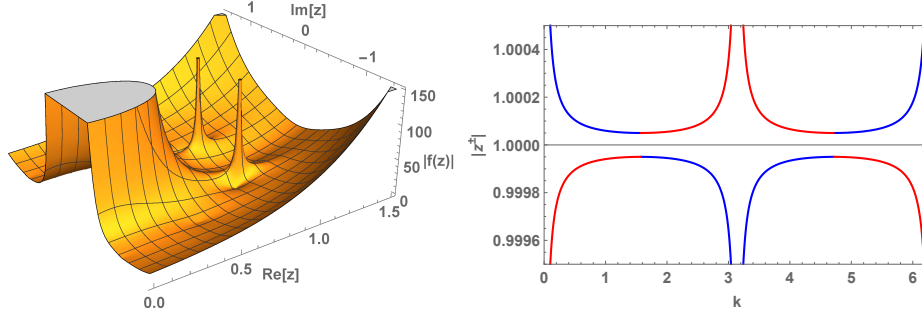
$$\left\langle n, \beta \left| \frac{1}{\epsilon_k - H_{\mathrm{res}}^{\beta} + i\eta} \right| 1, \beta \right\rangle = \frac{1}{\pi} \oint_{\mathcal{C}} \frac{\left(\frac{1}{2i}\right)^2 (z^n - \frac{1}{z^n})(z - \frac{1}{z})}{-2t(\cos(k) - \frac{z}{2} - \frac{1}{2z}) + i\eta} \frac{i}{z} \mathrm{d}z,$$

$$= \frac{i}{4\pi t} \oint_{\mathcal{C}} \frac{1}{z^{n+1}} \frac{(z^{2n} - 1)(z^2 - 1)}{2\cos(k)z - z^2 - 1 - \frac{i\eta}{t} z} \mathrm{d}z,$$

where $\mathcal{C}$ denotes the unit circle in $\mathbb{C}$. It is easy to see that the integrand has three poles, one at zero and two others at

$$z^{\pm} := \cos(k) - \frac{i\eta}{2t} \pm \sqrt{\left(\cos(k) - \frac{i\eta}{2t}\right)^2 - 1}.$$

Thus we can write rather compactly

$$\left\langle n, \beta \left| \frac{1}{\epsilon_k - H_{\mathrm{res}}^{\beta} + i\eta} \right| 1, \beta \right\rangle = \frac{i}{4\pi t} \oint_{\mathcal{C}} \frac{1}{z^{n+1}} \frac{(z^{2n} - 1)(z^2 - 1)}{(z - z^+)(z - z^-)} \mathrm{d}z =: \frac{i}{4\pi t} \oint_{\mathcal{C}} g(z) \mathrm{d}z.$$

Figure A.2: A plot of the moduli of g and $z^{\pm}$, left and right respectively (z^{+} in blue and z^{-} in red). The parameters were set to $n = 6$, $k = \pi/2$, $t = 1$ and $\eta = 10^{-6}$ (left) and $t = 1$ and $\eta = 10^{-4}$ (right).

As once can see in fig.A.2, only one of $z^{\pm}$ is in $\mathcal{C}$ at any time, and which one it is depends on k. Additionally one has to be wary of branch cuts when considering the limit $\eta \to 0^{+}$ in $z^{\pm}$. One can check (either numerically or by hand) that

$$
\begin{cases}
0 < k < \pi/2 : & z^{\pm} \to e^{\mp ik}, \ z^{-} \in \mathrm{Int}(\mathcal{C}) \\
\pi/2 < k < 3\pi/2 : & z^{\pm} \to e^{\pm ik}, \ z^{+} \in \mathrm{Int}(\mathcal{C}) \ . \\
3\pi/2 < k < 2\pi : & z^{\pm} \to e^{\mp ik}, \ z^{-} \in \mathrm{Int}(\mathcal{C})
\end{cases}
\tag{A.0.1}
$$

Thus it is our aim to compute

$$
\left\langle n, \beta \left| \frac{1}{\epsilon_k - H_{\mathrm{res}}^{\beta} + i\eta} \right| 1, \beta \right\rangle = -\frac{1}{2t} \left(\mathrm{Res}_0(g) + \mathrm{Res}_{z^{\pm}}(g) \right).
$$

An observation that will prove useful in simplifying the result is that $z^{+}z^{-} = 1$, independent of k, t and η.

We start with the residue at 0. Obviously g has a pole of order $n+1$ at the origin and so to compute the residue we need to find the Laurent expansion in some annulus enclosing 0. However, we can ignore the z^{2n} term, as it will not contribute to the terms we are interested in. We then expand

$$
\frac{1 - z^2}{z^{n+1}} \left[\frac{1}{(z - z^{+})(z - z^{-})} \right] = \frac{1}{z^{n+1}} \frac{1 - z^2}{z^{+} - z^{-}} \left[\frac{1}{z - z^{+}} - \frac{1}{z - z^{-}} \right],
$$

$$
= \frac{z^{-(n+1)}}{z^{+} - z^{-}} \sum_{j=0}^{\infty} \left(\left(\frac{1}{z^{-}} \right)^{j+1} - \left(\frac{1}{z^{+}} \right)^{j+1} \right) (z^j - z^{j+2}).
$$

From which we extract the term of order -1 and simplify (using $z^{+}z^{-} = 1$) to find

$$
\mathrm{Res}_0(g) = \frac{\left(\frac{1}{z^{-}} \right)^{n+1} - \left(\frac{1}{z^{+}} \right)^{n+1} - \left(\frac{1}{z^{-}} \right)^{n-1} + \left(\frac{1}{z^{+}} \right)^{n-1}}{z^{+} - z^{-}} = (z^{+})^n + (z^{-})^n.
$$

Now the residue at $z^{\pm}$, for this we use the technique of Lemma VI §1 1.3 from [12], this yields

$$
\mathrm{Res}_{z^{\pm}}(g) = \frac{((z^{\pm})^{2n} - 1)((z^{\pm})^2 - 1)}{(z^{\pm})^{n+1}(z^{\pm} - z^{\mp})} = (z^{\pm})^n - (z^{\mp})^n.
$$

Putting all of the above together we see that

$$
\left\langle n, \beta \left| \frac{1}{\epsilon_k - H_{\mathrm{res}}^{\beta} + i\eta} \right| 1, \beta \right\rangle = -\frac{1}{2t} \left(\mathrm{Res}_0(g) + \mathrm{Res}_{z^{\pm}}(g) \right) = -\frac{(z^{\pm})^n}{t},
$$

and noting from (A.0.1) that the root inside $\mathcal{C}$ always converges to e^{ik}, we find the desired result.

References

[1] Andergassen, S. , Pletyukhov, M. , Schuricht, D. , Schoeller H., and Borda L. *"A Renormalisation-Group Analysis of the Interacting Resonant Level Model at Finite Bias: Generic Analytic Study of Static Properties and Quench Dynamics"*. Phys. Rev. B 83, 205103 (2011).

[2] Anderson, P. *"Localized Magnetic States in Metals"*. Phys. Rev. 124, 41 (1961).

[3] Beenakker, C. W. J. and van Houten, H. *"Quantum Transport in Semiconductor Nanostructures"*. Solid State Physics, 44, 1-228, (1991).

[4] Bruus, H. and Flensberg, K. (2004). *"Many-Body Quantum Theory in Condensed Matter Physics"*. Oxford University Press, Oxford.

[5] Büttiker, M. *"Four-Terminal Phase-Coherent Conductance"*. Phys. Rev. Lett. 57, 1761 (1986).

[6] Datta, S. (1995). *"Electronic Transport in Mesoscopic Systems"*. Cambridge University Press, Cambridge.

[7] Esposito, M., Harbola, U. , and Mukamel S. *"Quantum Master Equation for Electron Transport through Quantum Dots and Single Molecules"*. Phys. Rev. B 74, 235309 (2006).

[8] Griffiths, D.J. (2005). *"Introduction to Quantum Mechanics"*, 2nd edition. Pearson Prentice Hall, Upper Saddle River.

[9] Imry, Y. (1997) *"Introduction to Mesoscopic Physics"*. Oxford University Press, Oxford.

[10] Kubo, R. *"Statistical-Mechanical Theory of Irreversible Processes. I."*. J. Phys. Soc. Jpn. 12, 570 (1957).

[11] Landauer, R. *"Spatial Variation of Currents and Fields Due to Localized Scatterers in Metallic Conduction"*. IBM J. Res. 1, 233 (1957).

[12] Lang, S. (1999). *"Complex Analysis"*, 4th edition. Springer Verlag, New York.

[13] Lippmann, B. and Schwinger, J. *"Variational Principles for Scattering Processes. I"*. Phys. Rev. 79, 469 (1950).

[14] Meir, Y. and Wingreen, N. *"Landauer Formula for the Current through an Interacting Electron Region"*. Phys. Rev. Lett. 68, 16 (1992).

[15] Roch, N. , Florens S. , Bouchiat V. , Wernsdorfer W. , and Balestro F. *"Quantum Phase Transition in a Single-Molecule Quantum Dot"*. Nature 453, 633-637 (29 May 2008).

[16] Schönauer, B. *"Nonlinear Quantum Transport in Nanoscopic Interacting Structures"*. Master Thesis, Karlsruhe Institute of Technology (2015).

[17] Shankar, R. (1994). *"Principles of Quantum Mechanics"*, 2nd edition. Springer Verlag, New York.

[18] Tuovinen, R., van Leeuwen, R., Perfetto, E. and Stefanucci, G. *'Time-Dependent Landauer-Büttiker Formula for Transient Dynamics'"*. Phys. Rev. B 89, 085131 (2014).

[19] van Ruitenbeek, J. M. *"Conductance Quantisation in Metallic Point Contacts"*. Appears as chapter 6 in: *"Metal Clusters on Surfaces: Structure, Quantum Properties, Physical Chemistry"*, K.-H. Meiwes-Broer, ed. (Springer-Verlag Berlin, 1999).

Acknowledgements