UNIVERSITY OF COPENHAGEN
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Master thesis

Field theory modelling of non-interacting junctions with induced potentials

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Abstract

Nanowires are an instrumental component of modern nano-technology and so a network of leads forming a star graph is considered. The leads are being modelled as being one dimensional, and we consider each channel within the lead to be induced by a potential, which physically is manifested as the energies of transverse modes in the lead. We consider arbitrary values of these induced potentials. At the vertex of the graph is a point-like and non-interacting general scatterer – and by finding a self-adjoint extension to the Hamiltonian, we are able to explicitly construct the unitary scattering matrix. The scattering matrix depend on the boundary conditions of the wavefunctions in each lead, as well as the energy of the incoming electron. By connecting each lead to a thermal reservoir, the system is away from equilibrium and it admits a non-equilibrium steady state.

Equipped with the scattering matrix formalism, we construct a quantum field theory on the star graph and calculate the electric current, particle density, differential conductance and the heat current. The x-dependence of the particle density is manifested as Friedel oscillations. Furthermore, the electric current is constant along edges, and thus the state constitute a steady state. Finally, we study the quantum quench protocol for switching from an equilibrium state without potentials, to suddenly enter a non-equilibrium regime and turning on the potentials.

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1 Introduction

Nanowires are quantum systems that can be approximated as being one dimensional and allow for transport of electrons. Nanowires are ubiquitous in modern nano-technology, and gaining insight in their inner workings is crucial. Nano-scale systems consisting of many nanowires leading to intersections are still a rarity, but fabricating such networks has been done in e.g. [1] and interesting physics emerges as a consequence, depending on the nature of the scatterer at the intersections.

Understanding nanowires is an essential prerequisite in the pursuit for realising many platforms for quantum technologies, and much effort has been put in studying and fabricating nanowires, since its experimental inception in 1991. The size of a usual nano-wire can typically be considered unrestricted in the longitudinal dimension, but severely confined along the transverse dimension down to less than 10 nanometers [2]. Due to this large length to width ratio, one considers this a quasi-one-dimensional system. The relative size of the transverse dimension usually allow for a multitude of conducting channels, within a single wire, to exist. The number of channels is partly determined by the conducting material's Fermi wavelength λ_F and the width (diameter for cylindrical wires or width of gate-induced nanowires in 2D semiconductors) w of the wire [2]. If $\lambda_F \gg w$, then many open channels (transverse modes) may exist, and when $\lambda_F \sim w$, few exist. A related structure that also hosts transverse modes is the nanotube, that contrary to the nanowire, is a hollow cylinder, where the shell is a layer of atom-thick graphene. This layer is then wrapped upon itself to create a hollow cylinder, whose diameter also is of order 10 nanometer. For hexagonal nanowires extending in the x direction, and by assuming discrete rotational symmetry, the wavefunction might look like $\psi_{\ell,k_x}(x,\varphi) = e^{i\varphi\ell}e^{ik_x x}R(\varphi)$ where $\varphi = (0, 2\pi]$ is the azimuthal angle, $\ell = 0, ..., 5$ accounts for the angular momentum, and $R(\varphi)$ is the radial dependence. For a given φ the wavefunction is invariant under $\varphi \to \varphi + 2\pi$ rotation, but will gain a phase for every $\pi/3$ turns, and this leads to transverse energies. The energy of the system is the sum of the transverse mode energies E_ℓ and the plane wave eigenenergy $E(k_x)$. The fact that one part of the energy depends on a parameter ℓ, allow us to, schematically, view this hexagonal nanowire as a network of 6 (independent) channels, one for each eigenvalue of the angular momentum $\ell = 0, ..., 5$. The same generalisation can be applied to the nanowire where dimensional confinement led to transverse modes. Each mode can be separated to its own lead, and we, get a network of non-interacting leads – one for each transverse mode. This is shown on figure 1.b.

For a general star graph of nanowires, we wish to set up a general framework for handling scattering phenomena with induced potentials in the wires. The formalism will encompass a large class of physical system, such as nanowires with discrete rotational symmetry, the gate-defined nanowires with transverse modes, nanotubes and the alike. By the same token, the general scatterer can represent a large family of physical system, like an impurity (magnetic or not), a quantum device, a region with a non-trivial spin orbit effect.

The simplest configuration of a nanowire-system is with two wires and a scatterer in the middle.

The two-terminal system has been explored in many papers, including the important [3] from 1985 and the experimental testing of the aforementioned paper in [4]. In it Büttiker et.al. show how, at non-zero temperature, the conductance across the junction depends on the reflection and transmission coefficient of the scattering matrix. Furthermore, they generalise the result to an arbitrary number of channels within each wire, although considering zero temperature. The system they studied can then be characterised as a multichannel system with just two terminal points (wires) and with each wire connected to a bath/reservoir, with differing chemical potentials. Systems of this nature with just two terminal points, is prevalent in the literature because of its simplicity, and ability to model a large class of junctions with an arbitrary number of channels.

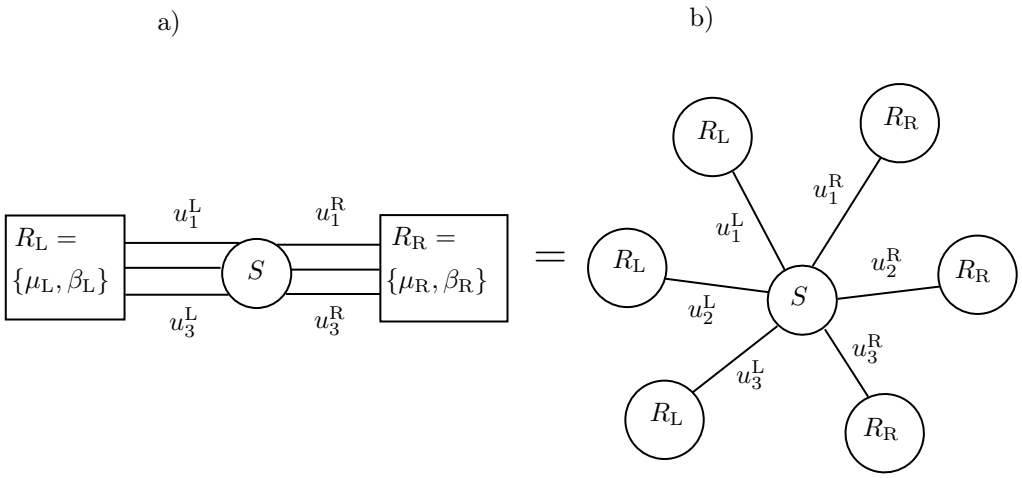


Figure 1: A two terminal device with transverse potential energies u can be mapped to a star graph, with each channel is associated with an induced potential $u_i^{\mathrm{L/R}}$ and reservoirs R_i. The reservoir is parameterised by a chemical potential $\mu_{\mathrm{L/R}}$ and an inverse temperature $\beta_{\mathrm{L/R}} = 1/T_{\mathrm{L/R}}$. The S at the vertex symbolises the point-like impurity/device, whose properties are characterised mathematically by the scattering matrix.

The star graph above is an approximate description of a large class of nano-structures, and thus much of this thesis will be devoted to understanding such quantum star graphs. Already, much research has been done on quantum star graphs by, e.g., M. Mintchev in [5]–[7]. There, non-equilibrium steady states and energy transmutation on quantum star graphs is studied respectively. What is always assumed though, is that the potentials in the leads are zero, meaning no transverse energies are present, only that the leads are connected to different reservoirs taking the system away from equilibrium. In this thesis, we also consider transverse energies (though constant), and we will show that observables such as electric current, particle density, conductance and heat current has very similar structure to those without potentials from [6]. However, we generalise the construction of the scattering matrix to account for general potentials.

Such a systems of nanowires is in general difficult to create in the laboratory, although there has been recent progress in making like [1], [8] both using Selective Area Growth to grow the wires. [1] created large networks of InAs semiconductor nanowires, which may at some point be used in a network of semiconductor-superconductor junctions. This is of course highly sought after, because of possibility of Majorana states, that could create fault-tolerant quantum computing, see also [8]. Even though complicated semiconductor heterostructures, nanotubes, molecules [9] are completely different, these nanostructures can be described by the same physics that we will discuss in this thesis.

The mathematical framework to describe quantum star graphs, is largely (at least in this thesis) contributed by V. Kostrykin and R. Schrader in [10]. The problem they study is the following: along each lead, each wavefunction is solely described by the Hamiltonian, that is hermitian – but at the vertex, the Hamiltonian is not sufficient, and a, so-called, self-adjoint extension to the Hamiltonian, is needed. This self-adjoint extension will depend on the boundary conditions of the wavefunctions at the vertex. This self-adjoint extension also lead to an explicit formula of the scattering matrix S that plays a central role.

In the following chapters, we will build the formalism for quantum star graphs with induced potentials, based on the papers by Mintchev et.al., [5], [6] and Kostrykin and Schrader [10]. The former built a quantum field theory and calculated observables, where the latter focused on a first quantisation method and include self-adjoint extensions of symmetric operators, and discuss symplectic forms. Then we will use the formalism and calculate the scattering matrix for two examples: the mixed Robin boundary conditions, and for a δ functions potential at the vertex. In chapter 5 we introduce quantum fields and calculate certain observables, like particle density, the electrical current and conductance. Lastly in chapter 6, we compare the two systems (with and without induced potentials) and see how one can evolve into the other through a sudden switch of the Hamiltonian. This will be an example of a quantum quench.

1.1 The Landauer-Büttiker formalism and Non-Equilibrium Steady States

These nano-systems are typically on the scale of nanometers or micrometers and in such systems, the properties are determined by both quantum mechanics and classical mechanics. One of the main observables one wants to know in a mesoscopic system is the electrical current and conductance. This is in general given by the Landauer-Büttiker formula, given that the electrons are not interacting, meaning the quantum mechanical coherence length must then by much greater than the size of the system. Such systems host unique transport properties that are different from those of bulk materials and individual atoms or molecules. For example, these systems can exhibit phenomena such as quantum interference, localisation, and universal conductance fluctuations. These phenomena arise from the fact that electrons in mesoscopic systems can be confined to small regions, and so their wave-like properties become important.

The usual setup is the one discussed earlier, with a scatterer in the middle and a set of chan-

nels/edges connected. Far away, those leads are then connected to metal contacts that supply an indefinite amount of electrons (the reservoirs). The assumptions on the reservoirs and the general coupling to the leads are as follows [3]: A reservoir is associated with a chemical potential μ, that is the maximum energy an electron that is emitted from the reservoir can have (at zero temperature). The reservoir emits electrons into the leads until all states in the lead are filled. An incident electron will get absorbed and thermalised – and the reservoir does not change. One can immediately find that if all reservoirs are equal, no current can run in any wire, and this situation is in thermal equilibrium. On the other hand, if the reservoirs are different, an electric current will flow. This current will in general depend on time and the position along the wire – but one finds that it indeed is constant along each wire, so the system is in an Non-Equilibrium Steady State (NESS).

To begin, we will review the simple case of only two terminal points, with no induced potential and state the Landauer-Büttiker formula for a two-terminal system.

1.1.1 The two terminal setup

The two terminal setup is a simple example on a nanowire/scattering setup which is the one with a scattering region and two leads connected to it. Far away, each lead is then connected to a reservoir with chemical potential μ_{L} and μ_{R}, and inverse temperature β_{L} and β_{R}.

Now, each lead is connected to its own reservoir with chemical potentials μ_{L} and μ_{R}. Much of this section is taken from [9], [11]. These two leads will get labelled with L for left and R for right lead, see again figure 1.a. Within each of these leads, are $2N$ channels, maybe originating from transverse modes discussed earlier. The setup is partly depicted on the left half of figure 1, although we will consider an arbitrary number of channels within each lead as opposed to only showing 3. Since there only are two leads, we can write the unitary scattering matrix as the following block matrix, that depend on the energy

$$\hat{S}(\varepsilon) = \begin{pmatrix} \hat{S}_{\mathrm{LL}}(\varepsilon) & \hat{S}_{\mathrm{LR}}(\varepsilon) \\ \hat{S}_{\mathrm{RL}}(\varepsilon) & \hat{S}_{\mathrm{RR}}(\varepsilon) \end{pmatrix} = \begin{pmatrix} r(\varepsilon) & t'(\varepsilon) \\ t(\varepsilon) & r'(\varepsilon) \end{pmatrix}. \tag{1.1}$$

Each sub-matrix $\hat{S}_i$, $i \in \{\mathrm{LL}, \mathrm{LR}, \mathrm{RL}, \mathrm{RR}\}$. Incoming electrons from the left have amplitudes r_{ij} and t_{ij} of being reflected and transmitted from channel j to i, and electrons coming from the left are likewise described by the primed matrices. The probability for right electrons to be transmitted or reflected from channel j to i is, respectively

$$T_{ij} = |t_{ij}|^2, \quad R_{ij} = |r_{ij}|^2. \tag{1.2}$$

The two reservoirs are filled according to a filling factor f_{L} and f_{R} for the left and right reservoir respectively. These filling factors depend on the temperature and chemical potential of the reservoirs, and will be the Fermi-Dirac distribution later.

We will now calculate current and also the conductance of such a two-terminal junction [3], [9]. Begin by assume $\mu_{\mathrm{L}} > \mu_{\mathrm{R}}$ such that the electrons are moving from left to right, and also define positive

momenta k by electrons moving away from the scattere. By taking a cross-section through the left lead we make the following observations: An electron with negative momentum $k < 0$ can only be coming from the left reservoir and is thus associated with filling factor f_{L}. A fraction of the electrons with positive momenta $k > 0$, will have been reflected at the scattere and the remaining fraction will have been transmitted to a reservoir with filling factor f_{R}. The fraction that have been reflected is $R_n = \sum_j R_{nj}$, and the transmitted fraction is $1 - R_n$ for channel n. The current is proportional to the sum (integral) of all momenta and channels, weighted by the Fermi velocity [9]. By change of variables and calculating the density of states $\mathrm{d}n/\mathrm{d}\varepsilon = 2/hv(k)$, one arrives at the Landauer equation for the electrical current:

$$I = \frac{e}{\pi}\int_0^\infty \mathrm{d}\varepsilon\, \mathrm{Tr}\big\{t^\dagger(\varepsilon)t(\varepsilon)\big\}\left(f(\varepsilon-\mu_{\mathrm{L}}) - f(\varepsilon-\mu_{\mathrm{R}})\right), \tag{1.3}$$

now with f being the Fermi-Dirac distribution

$$f(\varepsilon-\mu_{\mathrm{L/R}}) = \frac{1}{1+e^{\beta_{\mathrm{L/R}}(\varepsilon-\mu_{\mathrm{L/R}})}}. \tag{1.4}$$

One can then Taylor expand the electrical current I, by introducing the equilibrium chemical potential μ as $\mu_{\mathrm{L/R}} = \mu - eV_{\mathrm{L/R}}$, and then expanding in eV_{L} and eV_{R} around μ. One get [11], with Planck's constant h explicitly inserted that

$$I \approx -\frac{e^2}{h}\int_0^\infty \mathrm{d}\varepsilon\, \mathrm{Tr}\big\{t^\dagger(\varepsilon)t(\varepsilon)\big\}\frac{\partial f(\varepsilon-\mu)}{\partial\varepsilon}(V_{\mathrm{L}} - V_{\mathrm{R}}) \tag{1.5}$$

and by $G = I/(V_{\mathrm{L}} - V_{\mathrm{R}})$, as well as assuming zero temperature $\partial f/\partial\varepsilon = -\delta(\varepsilon-\mu)$

$$G(\mu) = \frac{2e^2}{h}\,\mathrm{Tr}\big\{t^\dagger(\mu)t(\mu)\big\}. \tag{1.6}$$

The conductance is then only a function of the equilibrium chemical potential, and we have also assumed that the spin degree of freedom is degenerate, hence the factor of 2.

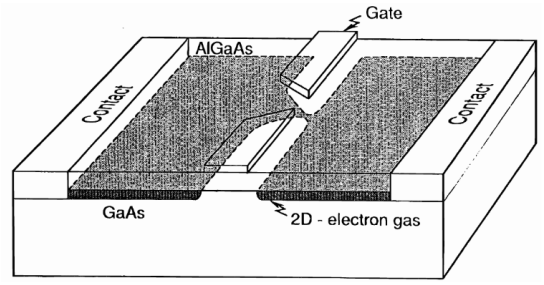
This system is clearly not in an equilibrium state, as there is an exchange of particles with external reservoirs. This is by assuming that $\mathrm{Tr}\, t^\dagger t \neq 0$, since if there was no transmission between edges with different reservoirs, one would exist in an equilibrium state. This can be generalised from two reservoirs to N by the unitary scattering matrix S. If S admits non-zero transmission amplitudes between non-equal reservoirs, the system is away from equilibrium [6]. And as the current in (1.3) and hence the conductance, among other observables, are time-independent, this is a Non-Equilibrium Steady State (NESS).

Experimental work on quantised conductance

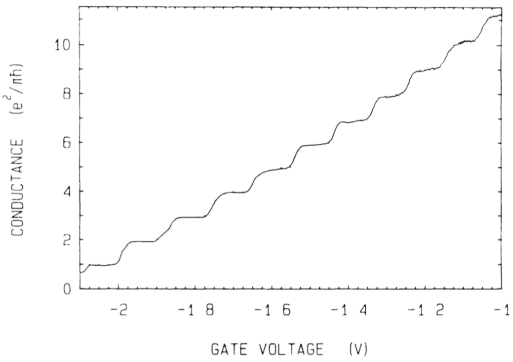
Experimentally this has been demonstrated a multitude of times, the first being in 1988 by [4]. The authors found that the conductance is indeed quantised in integer values of $G_0 = 2e^2/h$, called the conductance quanta. Since the conductance is given by the trace of $t^\dagger t$, the larger this matrix is, the larger, in general, the conductance is. The dimension of $t^\dagger t$ depends on the number of open channels that allow electron transmission through the scatterer. For a given energy E, a channel is only open

if E is greater than the potential in the channel, and so by increasing the energy, one opens more channels. The following experiment is two-dimensional setup and using a two-dimensional electron gas (2DEG), so the formalism we study in this thesis will not be applicable to describe such systems. The system can be brought to one-dimensional by simply squeezing the transverse dimension as seen in figure 2a, such that the "Contacts" only have a single point of contact to the wires (2DEG).

The way [4] modelled the scatterer was by a so called split-gate technique [9], [11]: They employed GaAlAs-GaAs semiconductor heterostructur which forces the electrons to the surface of the GaAlAs layer, and thus by placing a set of metallic gate electrodes top of the heterostructure, one is able to control the number of open channels in the 2DEG. This is done simply by varying the voltage across the metal electrodes, confining the width of the potential in the wire, that allow transport. Thus by varying the voltage, new channels open, and the conductance jump in a step of G_0. The number of open channels is $\lfloor k_F a_{\min}/\pi \rfloor$, where k_F is the Fermi wave number and $a_{\min}$ is the narrowest point of the confinement created by the electrodes. One can also conclude that the staircase-like graph formed when varying the gate-voltage and measuring the conductance, is a really "sharp" staircase when the system is entirely classical, meaning either transmission and reflection is either 0 or 1; the quantum mechanical behaviour is manifested when it takes on values in-between. The experimental setup (from another paper) as well as the historical observed conductance is shown below on figure 2a and 2b respectively.



(a) Figure showing a similar experimental setup as the original one performed by [4]. The figure is from [12].



(b) Conductance across a two terminal device as a function of the gate voltage. The conductance is in clear steps of the conductance quantum G_0. From [4].

Figure 2

Another way to induce non-equilibrium is by a quantum quench protocol. Here one temporally transitions from a state in equilibrium to a state not in equilibrium. This sudden change leaves the system in a transient state after which it may settle to a steady state again. One may also do the opposite. And we will study both cases in more detail.

1.2 Quantum quenches

After building the formalism for both induced potentials and without, we will see the connection between the two, by the protocol of a quantum quench. A quantum quench is a protocol in which a quantum system, with initial Hamiltonian H_i evolves in its eigenstate until a specific time $t = t_0$ where, suddenly (or gradually) a parameter in the system change, and the Hamiltonian changes accordingly. Thus the system evolves according to a new, final, Hamiltonian H_f. One is then interested in how physical observables change, as well. This is often a non-trivial calculation, since expectation values of operators in a state which is not an eigenstate may prove difficult. Specifically, we will see how the average current changes after a quench, and if it settles into a steady state.

In [13] the authors compare different physical theories of calculating the average current in the following setup: two 1D lattices are connected through a non-interacting junction. The two methods considered are the LB scattering procedure and the Micro-Canonical Formalism (MCF). The authors consider two quench protocols which will be very similar to the ones we will be considering in section 6. **The density quench**: at time $t < 0$, the leads are disconnected to the junction, and a voltage bias is present in the leads, such that the density is the leads are not equal. At $t \geq 0$ the leads are connected to the junction and the voltage bias across each leads is removed. $\boldsymbol{\mu}$ **quench**: At time $t < 0$, the leads are connected to the junction, without a voltage difference. At $t \geq 0$, a voltage is created in each lead, and the densities are different, so a current flows through the junction.

The MCF assumes a closed system with a finite and constant number of particles – contrary to the LB scheme, where an open system, with infinitely long wires, and an indefinite number of particles which can be supplied from thermal reservoirs, is assumed. Either way, the authors find that the two schemes agree largely on the average current, for semi-large times. An interesting feature they find for the LB system, is that the particles at the reservoirs need not obey Fermi-Dirac statistics. Analysis on density vs μ quench has been done in [13], [14]. In addition, [15] analysed the density quench with a hydrodynamic approach.

One may also consider a slow quench, in which one adiabatically turn on parameters that turn a simple Hamiltonian into a complicated one, whose ground state in the sought after. We will rather consider a sudden quench, in which one inject a large amount of energy into the system, and thus the ground-state is no longer an eigenstate for the system. Even though the voltage in wires usually oscillate much slower than the motion of electrons, a sudden quench is a good approximation in the long-time limit.

Previously we looked at the simplest case of a scattering matrix: the two-terminal setup without induced potentials. We will now introduce the scattering matrix more rigorously, and to begin with, assume no induced potentials in the leads. In section 3, we introduce the potentials and will explore the implications the potentials cause.

2 The Schrödinger junction without induced potentials

In this section, we will succinctly recap known results, taken from [5], [10], where a quantum star graph with N edges, all connected at a vertex V, is being studied. We will start by studying the bulk of the graph: $G\backslash V$, i.e. what fields propagate on the edges, and the section that follows will then contain the physics at the vertex V, i.e. the scattering matrix.

2.1 Fields in the bulk

The system we wish to explore is the one depicted on figure 3. N independent edges connected to a single vertex. There is no induced potential in any channel, and we assume the leads are perfect conductors in the sense that there is no energy loss due to dissipation.

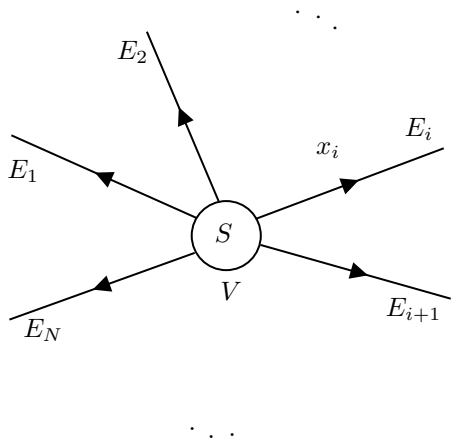


Figure 3: Inspired by [5]. Shows the graph G along with its N edges all with $x_i > 0$ for all $i = 1, ..., N$, as well as the vertex V located at $x = 0$. This is also the location of the point-like scatterer, that is represented by a scattering matrix S.

The dynamics of the system is a simple scattering process: we inject an electron wave into edge E_i and we want to describe its scattering properties in other edges. We can describe the system by a state vector $|\chi_a(\varepsilon)\rangle$, where a labels which channel we inject a wave into, and ε is its energy. With H^0 being the Hamiltonian

$$H^0 |\chi_a(\varepsilon)\rangle = \varepsilon |\chi_a(\varepsilon)\rangle , \tag{2.1}$$

Where $\varepsilon > 0$. If we let b label which specific channel we're probing and x be the distance from the vertex on edge E_b, the combination of the two, fully describes positions on $G\backslash V$. We assume the state $|b, x\rangle$ is an orthonormal basis, i.e.

$$1 = \int_0^\infty \mathrm{d}x \sum_{b=1}^{N} |b, x\rangle \langle b, x| , \tag{2.2}$$

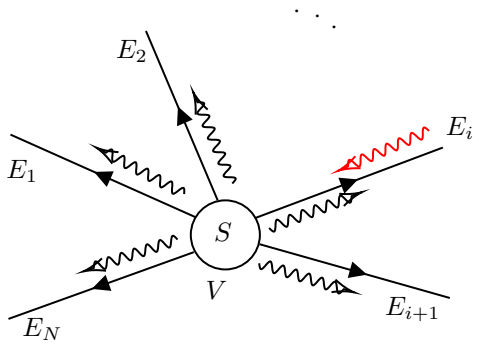
where 1 here symbolises an identity operator. In the bulk i.e. for $x > 0$, the particles are free, and since $\langle b', x' | H | b, x \rangle = -\delta_{bb'}\delta(x - x')\partial^2_{b,j}/2m$. So the Hamiltonian on edge E_j is given by

$$H_j^0 = -\frac{\partial^2_{j,x}}{2m}, \quad m > 0, \tag{2.3}$$

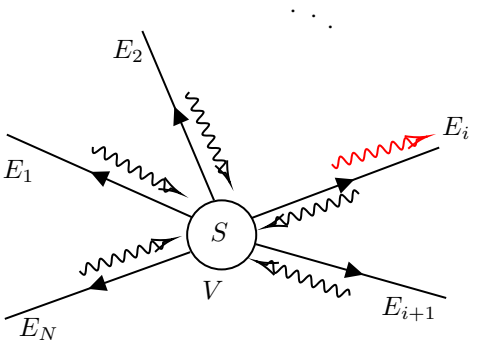
where m is the electron mass and $\langle b, x | \chi_{ab}(\varepsilon) \rangle = \chi_{ab}(x, \varepsilon)$ is the electronic wavefunction where a labels the channel of the incoming particle, and b is which lead we're probing. The j index on the derivative is to explicitly state that the derivative only acts on edge E_j, but will often get suppressed. The Hamiltonian in the bulk of the graph is

$$H^0 = \bigoplus_{j=1}^{N} H_j^0 = \bigoplus_{j=1}^{N} \frac{-\partial^2_{j,x}}{2m}, \tag{2.4}$$

Where the direct sum is taken over all N channels. For the following of the thesis, we assume each lead is a perfect one-dimensional conductor with no impurities, such that each wave is a plane wave. Furthermore, all electrons are completely incoherent, and do not interact. We now have a choice between a basis of the wavefunctions: either we insert a wave in lead i that then gets transmitted into the remaining $N - 1$ edges, and reflected back in i by the scatterer at the vertex – or waves from all edges meet at the vertex and culminate to a single wave in just lead i. These two scenarios are basis 1 and 2 and are depicted on figure 4a and 4b, respectively. They are physically equivalent, and both constitute an orthonormal basis, and so there exists a unitary transformation between the two. We will see in section 5.1 that this transformation simply is given by the scattering matrix S. We will use basis 1 in the following.



(a) Basis 1 takes *incoming* waves to the junction to be e^{-ikx}, $k > 0$.



(b) Basis 2 takes *outgoing* waves from the junction to be e^{-ikx}, $k < 0$.

Figure 4: The graph G with the two bases shown. The two wavefunction bases. The filled black arrows on each lead shows which way positive x is.

The two plane waves that can exist on edge E_i is the plane wave e^{-ikx}, $x, k > 0$ with amplitude unity if it originates from $x = +\infty$, and a rescaled version Ae^{-ikx} if it has been scattered from the vertex. We will find that the prefactor A is elements of the scattering matrix. Since there are no induced potentials, the leads are identical and momentum is conserved across the junction. We assume in the remaining that the scattering matrix acts as a non-interacting junction, such that we are allowed to only consider a single electron at a time. So S will in general depend on the momentum k of the particle that is to get scattered: $S(k)$. We will assume that S can scatter to and from all N edges, hence S is $N \times N$. The entries of the matrix $S_{ab}(k)$, $a \neq b$ has the simple interpretation of probability amplitude of a particle coming from edge E_b, and getting scatted to edge E_a, i.e. transmission amplitudes, and so the diagonal elements $a = b$ are reflection amplitudes. To conserve probability current, one requires the scattering matrix to be unitary, i.e.

$$S^\dagger(k)S(k) = \mathbf{1}_N, \tag{2.5}$$

where $\mathbf{1}_N$ is the $N \times N$ identity matrix. The wavefunctions that propagate in the bulk of the graph $G\backslash V$ is

$$\chi_{ab}(x,k) = e^{-ikx}\delta_{ba} + e^{ikx}S_{ba}(k), \quad x, k > 0. \tag{2.6}$$

We have renamed the wavefunction's dependence on energy ε to momentum k. Here the labels a and b both range from $a, b \in [1, N]$ and k is the momentum of the electron[1]. These wavefunctions are eigenfunctions to the Hamiltonian in (2.3):

$$H_b^0\chi_{ab}(x,k) = \frac{k^2}{2m}\chi_{ab}(x,k) \tag{2.7}$$

hence the eigenenergy is

$$\varepsilon = \frac{k^2}{2m}. \tag{2.8}$$

It has been shown in [5] that the wavefunctions are orthogonal

$$\int_0^\infty \mathrm{d}x \sum_{b=1}^{N} \chi^*_{a'b}(x,k')\chi_{ab}(x,k) = 2\pi\delta_{aa'}\delta(k-k'). \tag{2.9}$$

Furthermore, they form a complete set if there are no bound states at the vertex meaning

$$\int_{-\infty}^\infty \frac{\mathrm{d}k}{2\pi} e^{ikx}S_{ba}(k) = 0, \tag{2.10}$$

then

$$\int_0^\infty \mathrm{d}k \sum_{a=1}^{N} \chi^*_{ab'}(x',k)\chi_{ab}(x,k) = 2\pi\delta_{bb'}\delta(x-x'). \tag{2.11}$$

This section was limited to the physics in the bulk of the graph. In the following we will study how the scattering matrix, at the vertex plays a role. We will find a closed matrix-equation for S as a function of the momentum and the boundary condition that the wavefunction make at the vertex.

[1]We have set $\hbar = 1$ and Boltzmann's constant $k_\mathrm{B} = 1$ throughout the thesis

2.2 Self-adjoint extensions and the scattering matrix

We will now discuss in more detail the actual structure of the scattering matrix S. Much of the following is taken from [5], [10], [16]. Given two quantum states ψ and ϕ on a quantum star graph G with N edges connected at the vertex V, we can define the following vector

$$\psi(x) = (\psi_1(x), \cdots, \psi_N(x))^\top \tag{2.12}$$

and likewise for ϕ. Each component ψ_i lives on edge E_i and belong to the Hilbert space

$$\mathcal{H}_i = L^2([0, \infty[). \tag{2.13}$$

Thus the Hilbert space for the graph G is

$$\mathcal{H}_G = \bigoplus_{i=1}^{N} \mathcal{H}_i = \bigoplus_{i=1}^{N} L^2([0, \infty[), \tag{2.14}$$

with the states $\psi, \phi \in \mathcal{H}_G$. An inner product over $\mathcal{H}_G$ is defined as

$$\langle \psi, \phi \rangle_{\mathcal{H}_G} = \sum_{i=1}^{N} \langle \psi_i, \phi_i \rangle_{\mathcal{H}_i} = \sum_{i=1}^{N} \int_0^\infty \mathrm{d}x \; \psi^*(x)\phi(x), \tag{2.15}$$

where * is complex conjugation. The inner will be written from now on simply as $\langle \psi, \phi \rangle$. We require self-adjointness of the Hamiltonian given in (2.3)

$$\langle \psi, H\phi \rangle = \langle H\psi, \phi \rangle, \quad \forall \psi, \phi \in \mathcal{H}_G. \tag{2.16}$$

Our task is then to find which boundary conditions (BC) we must enforce to have self-adjointness. With the shorthand notation

$$\partial_x \phi_i(0) = \lim_{x \to 0^+} \partial_x \phi_i(x), \tag{2.17}$$

$$\phi_i(0) = \lim_{x \to 0^+} \phi_i(x) \tag{2.18}$$

for any $i = 1, ..., N$, we find, by assuming the fields vanish as $x \to \infty$, and using partial integration

$$\langle \psi, H\phi \rangle = \sum_{i=1}^{N} \int_0^\infty \mathrm{d}x \; \psi_i^*(x) \frac{-\partial_x^2}{2m} \phi_i(x) \tag{2.19}$$

$$= \frac{1}{2m} \sum_{i=1}^{N} \Big[\psi_i^*(0)\partial_x \phi_i(0) - \partial_x \psi_i^*(0)\phi_i(0) \Big] + \langle H\psi, \phi \rangle, \tag{2.20}$$

so the BC becomes

$$\sum_{i=1}^{N} \psi_i^*(0)\partial_x \phi_i(0) = \sum_{i=1}^{N} \partial_x \psi_i^*(0) \; \phi_i(0). \tag{2.21}$$

The above equation is a direct consequence of the requirement of self-adjointness of the Hamiltonian in the bulk. It has been shown in [10] that the self-adjoint extension to H on the boundary is uniquely

defined by the following three conditions for A and B given by $N \times N$ matrices

$$A\psi(0)+B\psi'(0) = 0, \tag{2.22a}$$

$$AB^\dagger = BA^\dagger, \tag{2.22b}$$

$$\text{the composite } N \times 2N \text{ matrix } (A, B) \text{ has maximal rank } N. \tag{2.22c}$$

There exists equivalent conditions for the state ϕ. That is to say, these three equations maximise the Hilbert space in which (2.21) holds. The prime on $\psi'(x)$ denotes the derivative with respect to position x. We will see later that $\psi(x)$ is an annihilation operator in second quantisation, and will be discussed in section 5, in more detail. The components $\psi_b(x)$ for $b \in [1, N]$ of the field $\psi(x)$ is given by

$$\psi_b(x) = \int_0^\infty \frac{\mathrm{d}k}{2\pi} \sum_{a=1}^{N} \chi_{ab}(x, k)c_a(k), \tag{2.23}$$

with $c_a(k)$ being fermionic operators in lead a with momentum k, and satisfy anti-commutation-relations. From (2.22a), we get, with the wavefunction χ_{ab} given by 2.6, that

$$\sum_{j=1}^{N}(A_{bj}\psi_j(0) + B_{bj}\psi'_j(0)) = 0, \quad \forall b = 1, ..., N \tag{2.24a}$$

$$\int \frac{\mathrm{d}k}{2\pi} \sum_{a=1}^{N} c_a(k) \sum_{j=1}^{N} [A_{bj}\chi_{aj}(0, k) + B_{bj}\partial_x\chi_{aj}(x, k)|_{x=0}] = 0 \tag{2.24b}$$

The solution to the equation $C = \sum_a c_a v_a = 0$ for c_a an annihilation operator and $v_a \in \mathbb{C}$ makes sense if one considers C acting on all vectors. If one does not consider the vacuum state $|0\rangle$, the general solution is that $v_a = 0$, $\forall a$, as $c_a |0\rangle = 0$. So

$$\sum_{j=1}^{N} (A_{bj}\chi_{aj}(0, k) + B_{bj}\partial_x\chi_{aj}(x, k)|_{x=0}) = 0, \quad \forall a, b = 1, ..., N \tag{2.25a}$$

$$A_{ba} - i(Bk)_{ba} + (AS)_{ba} + i(BkS)_{ba} =0, \quad \forall a, b, = 1, ..., N. \tag{2.25b}$$

and so the scattering matrix in matrix form is

$$S(k) = -(A + iBk)^{-1}(A - iBk). \tag{2.26}$$

where here $k \in \mathbb{R}$. The existence of the inverse $(A + iBk)$ has been proved in [10]. By the rewriting

$$S(k) = -\left(A^\dagger - iB^\dagger k\right)\left[AA^\dagger + k^2 BB^\dagger\right]^{-1}(A - iBk) \tag{2.27}$$

and by using (2.22b), we see that the matrix is unitary and satisfy

$$S^\dagger(k) = S(-k), \tag{2.28}$$

and by their combination, we get

$$S(k)S(-k) = 1. \tag{2.29}$$

An important note of the scattering matrix, is that it is not possible to explicitly write out the elements S_{ab} explicitly as functions of k A_{ab} and B_{ab}.

Generally the scattering matrix depend on the momentum k of an incoming electron wave, but there exists special cases where $S(k)$ may be k-independent. This is the case if we let a matrix $C(\lambda)$ for $\lambda > 0$ exist, such that $C(\lambda)A = A$ and $C(\lambda)B = \lambda B$, [10]. The independence of k can be seen by multiplying (2.22a) by $C(\lambda)$ from the left, and then one get $A\psi(0) + B\lambda\psi'(0) = 0$, simply meaning $B \to \lambda B$, and if that happens to (2.26), one get the same equation but with $k \to \lambda k$, meaning $S(k)$ cannot depend on k. This is an important feature, only of the non-induced leads. The wavefunction $\psi_b(x)$ has units of $1/\sqrt{\mathrm{L}}$ where L is a length. We choose A to be unit-less and B has then units of length, in arbitrary units. We will now consider leads with induced potentials.

3 The Schrödinger junction with induced potentials

We now introduce the induced potentials $U_j(x)$ in each edge E_j. The potential $U_j(x)$ can in general have a non-trivial dependence on position along the edge x, as well as the collection of all the chemical potentials at the reservoirs. These potentials can originate from a multitude of reasons, and the following is a non-exhaustive list:

1. The potential $U_j(x)$ in channel j can be induced from a neighbouring electrostatic gate that is in proximity of the wire, i.e. they are coupled capacitively. This technique has been done in e.g. [17].

2. Induced potential $U_j(x)$ in channel j can be inherited directly from the reservoirs themselves. Calculating this effect would be done by solving the Schrödinger-Poisson equations self-consistently: The potential in lead $j = 1, ..., N$ solve Poisson's equation

$$\nabla^2 U_j(x) \propto N_0 - n_j(x) \tag{3.1}$$

where N_0 is a background density of electrons, corresponding to the Fermi energy. And

$$n_j(x) = \int_{-\infty}^{\infty} \mathrm{d}\varepsilon \sum_{a \text{ open}} |\chi_{aj}(x,\varepsilon)|^2 f_a(\varepsilon - \mu_a) \tag{3.2}$$

is the density of electrons in lead j, $f_a(\varepsilon - \mu_a) = (\exp(\beta_a(\varepsilon - \mu_a)) + 1)^{-1}$ is the Fermi-distribution at reservoir R_j with chemical potential μ_a and inverse temperature $\beta_a = 1/T_a$ and $\chi_{aj}(x,\varepsilon)$ is the wavefunction that satisfy the Schrödinger equation

$$\left(-\frac{\partial_x^2}{2m} + U_j(x)\right)\chi_{aj}(\varepsilon, x) = \varepsilon_j \chi_{aj}(x,\varepsilon) \tag{3.3}$$

where ε_j is the eigenenergy of edge E_j, that in general may differ from each edge. This description is purely physical and will happen regardless or not, though the potentials induced by this effect might be small.

In the following, we will make the simplistic assumption that the potential in edge E_j, $U_j(x) = U_j$ is constant.

For the formalism in the previous section without potentials, we had shifted the energy-scale up by the Fermi-energy such that the ground-state had zero particles, but in this case, we now include it explicitly, since a constant shift in the Fermi-energy for different leads, may be thought of as leads with different Fermi-energies all together. We are considering metallic leads with a Fermi energy of $\mathcal{E}_{\mathrm{F}} > 0$. So for a constant induced potential U_j across channel E_j the Hamiltonian in channel E_j is

$$H_j = \frac{-\partial_x^2}{2m} + U_j - \mathcal{E}_{\mathrm{F}}. \tag{3.4}$$

We define the quantity

$$u_j \equiv U_j - \mathcal{E}_{\mathrm{F}}, \tag{3.5}$$

and will from now on rename this the induced potential. A schematical depiction of the situation is on figure 5.

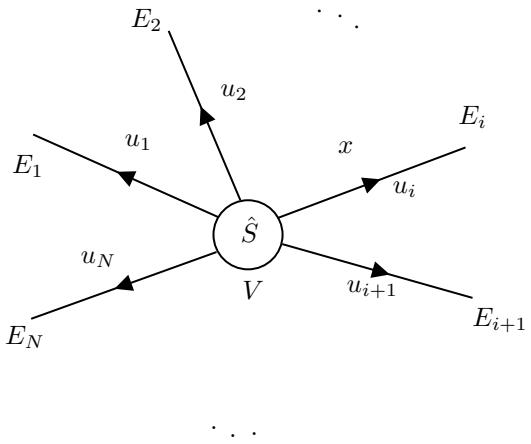


Figure 5: The graph G with N edges and a vertex V at $x = 0$. At each edge E_i is a constant potential u_i. The usual unitary scattering matrix S is replaced by $\hat{S}$, which is a consequence of the non-zero potentials u in the leads.

3.1 Fields in the bulk with induced potentials

First we will introduce the notion of open and closed channels. These are an artefact of the induced potentials: consider the edge E_j with associated potential u_j. Only particles with energy $\varepsilon > u_j$ may exist, so for given ε only a subset of all leads are open:

- **Open channel:** For a fixed ε and a fixed set of potentials $\boldsymbol{u} = \{u_1, \cdots, u_N\}$, an open channels/edge E_i with an associated potential u_i satisfies $\varepsilon > u_i$. The number of open channels is denoted n and is the size of the set of open channels

$$\mathcal{O}(\varepsilon) = \{j,\ \varepsilon - u_j > 0\}, \tag{3.6}$$

so

$$n = n(\varepsilon) = \#\mathcal{O}(\varepsilon) \tag{3.7}$$

with $\#A$ denoting the number of elements in the set A.

- **Closed channel:** For a fixed ε, a closed channels E_i with induced potential u_i satisfies $\varepsilon \leq u_i$. By the same token, the number of closed channels η depend on ε as

$$\mathcal{C}(\varepsilon) = \{j,\ \varepsilon - u_j \leq 0\}, \tag{3.8}$$

and

$$\eta = \eta(\varepsilon) = N - n(\varepsilon), \tag{3.9}$$

with N being the total number of edges in the system.

In the light of the possibility of a channel being open or closed, $|\chi_a(\varepsilon)\rangle$ might not be an eigenstate to H for $a = 1, ..., N$, but

$$H\,|\chi_a(\varepsilon)\rangle = \varepsilon\,|\chi_a(\varepsilon)\rangle\,, \quad a \in \mathcal{O}(\varepsilon). \tag{3.10}$$

and by inserting $1 = \int \mathrm{d}x' \sum_{b'} |b', x'\rangle \langle b', x'|$, and multiplying with $\langle b, x|$, we find

$$\int_0^\infty \mathrm{d}x' \sum_{b'=1}^{N} \langle b, x|\, H\, |b', x'\rangle\, \chi_{ab'}(x', \varepsilon) = \varepsilon \chi_{ab}(x, \varepsilon) \tag{3.11}$$

with $\chi_{ab}(x, \varepsilon) = \langle b, x|\chi_a(\varepsilon)\rangle$. By incorporating the induced leads, the Hamiltonian on edge E_j is

$$H_j = -\frac{\partial_x^2}{2m} + u_j \tag{3.12}$$

and so the Hamiltonian on $G\backslash V$ is

$$H = \bigoplus_{j=1}^{N} H_j = \bigoplus_{j=1}^{N} \left(-\frac{\partial_x^2}{2m} + u_j \right) \tag{3.13}$$

So from above we find

$$H_b \chi_{ab}(x, \varepsilon) = \varepsilon \chi_{ab}(x, \varepsilon) \tag{3.14}$$

the eigenenergy is

$$\varepsilon = \frac{k_i^2}{2m} + u_i, \tag{3.15}$$

for any $i = 1, ..., N$, that, contrary to the case with no induced potentials, does not have momentum conserved across the junction, though the energy ε is. This changes the dependence of the wavefunction and the scattering matrix, from k to ε as

$$\chi_{ab}(x, \varepsilon) = e^{-ik_a(\varepsilon)x}\delta_{ba} + e^{ik_b(\varepsilon)x} S_{ba}(\varepsilon), \quad x > 0,\ a \in \mathcal{O}(\varepsilon). \tag{3.16}$$

where in general

$$k_j(\varepsilon) = \sqrt{2m(\varepsilon - u_j)}. \tag{3.17}$$

In the case of $\varepsilon - u_j < 0$, we are left with an evanescent wavefunctions in channel E_j, hence no electronic transport. We introduce a new notation for such a number and will from now on suppress the energy-dependence on $k_j(\varepsilon)$ and simply write k_j. We define

$$k_j = \sqrt{2m(\varepsilon - u_j)} = \theta(\varepsilon - u_j)\sqrt{2m(\varepsilon - u_j)} + i\theta(u_j - \varepsilon)\sqrt{2m(u_j - \varepsilon)} \tag{3.18}$$

where $\theta(x)$ is the Heaviside step function that takes the value 1 if $x > 0$ and 0 if $x \leq 0$, and we define

$$k_j^o = \theta(\varepsilon - u_j)\sqrt{2m(\varepsilon - u_j)} \tag{3.19a}$$

$$k_j^c = \theta(u_j - \varepsilon)\sqrt{2m(u_j - \varepsilon)} \tag{3.19b}$$

$$k_j = k_j^o + ik_j^c, \quad k_j^o k_j^c = 0. \tag{3.19c}$$

The superscripts o and c are short for *open* and *closed*. Since the numbering of the leads is arbitrary, we have let

$$u_1 \leq u_2 \leq \cdots \leq u_N. \tag{3.20}$$

The momentum in (3.19) can be listed as the entries in an $N \times N$ non-invertible diagonal matrix as

$$\boldsymbol{k}^o = \mathrm{diag}\Big(k_1^o, \cdots, k_n^o, \underbrace{0, \cdots, 0}_{\eta}\Big), \quad \boldsymbol{k}^c = \mathrm{diag}\Big(\underbrace{0, \cdots, 0}_{n}, k_{n+1}^c, \cdots, k_{n+\eta}^c\Big) \tag{3.21}$$

with $n + \eta = N$ being the total number of leads in the system. The momentum k still depends on the energy ε, and so does n, meaning the rank of $\boldsymbol{k}^o$ and $\boldsymbol{k}^c$ depends on ε. The $N \times N$ momentum matrix $\boldsymbol{k}$, is thus

$$\boldsymbol{k} = \mathrm{diag}\Big(k_1^o, \cdots, k_n^o, ik_{n+1}^c, \cdots, ik_N^c\Big). \tag{3.22}$$

The momentum matrix $\boldsymbol{k}$ is not invertible at specific values of ε, indeed it has a single zero on the n'th entry: $k_i(u_i) = 0 \ \forall i = 1, ..., N$. So $\boldsymbol{k} = \boldsymbol{k}(\varepsilon)$ is invertible on the values $\varepsilon \in \mathbb{R}\backslash\{u_1, ..., u_N\}$, and if $\varepsilon < u_1$, then all channels will be closed, and $\boldsymbol{k}$ is purely imaginary. Likewise, if $\varepsilon > u_N$, then all channels are open and $\boldsymbol{k}$ is real. This almost invertibility will get discussed further once the unitary scattering matrix $\hat{S}$ is introduced.

Taking the possibility of closed channels into consideration, we generalise the wavefunction as

$$\chi_{ab}(x, \varepsilon) = \sqrt{v_a^o}^{-1}\left(e^{-ik_a^o x}\delta_{ba} + e^{i(k_b^o + ik_b^c)x}S_{ba}(\varepsilon)\right), \quad x > 0, \ a \in \mathcal{O}(\varepsilon) \tag{3.23}$$

with units of $1/\sqrt{\mathrm{L} \cdot E}$ with L being length and E energy, both in arbitrary units, and the scattering matrix is unit-less. We also introduced the (Fermi) velocity

$$v_a^o = \frac{\partial \varepsilon}{\partial k_a^o} = \frac{k_a^o}{m} \tag{3.24}$$

Furthermore, we included the normalisation constant $1/\sqrt{v_a^o}$, such that the following orthogonality relation holds:

$$\int_0^\infty \mathrm{d}x \sum_{b=1}^{N} \chi_{a'b}^*(x, \varepsilon')\chi_{ab}(x, \varepsilon) = 2\pi\delta_{aa'}\delta(\varepsilon - \varepsilon'), \tag{3.25}$$

which has been proven in Appendix C. The primed variables only refer to a different energy, and the potentials in each wire is the same is both cases. So

$$k_j^o = \theta(\varepsilon - u_j)\sqrt{2m(\varepsilon - u_j)}, \tag{3.26}$$

$$k_j^{o\prime} = \theta(\varepsilon' - u_j)\sqrt{2m(\varepsilon' - u_j)}, \tag{3.27}$$

likewise for k_j^c and so

$$\chi^*_{a'b}(x,\varepsilon') = \sqrt{v_{a'}^{o\prime}}^{-1}\left(e^{ik_{a'}^{o\prime}x}\delta_{ba'} + e^{-i(k_b^{o\prime}-ik_b^{c\prime})x}S_{ba'}(\varepsilon')\right). \tag{3.28}$$

Since ε and ε' in general are not equal, and they dictate the number of open channels $n = n(\varepsilon)$ and $n' = n(\varepsilon')$

$$1 \le a' \le n', \quad 1 \le a \le n, \tag{3.29}$$

we assume the following

$$\varepsilon' > \varepsilon, \quad n' \ge n, \tag{3.30}$$

where the equality $n' = n$ is true when there is at least one intermediate u_i making $\varepsilon' - \varepsilon < u_i - u_{i-1}$.

This section was limited to the physics of the bulk of the graph. We will now explore the vertex when the edges are induced. This follows the procedure of section 2.2 closely.

3.2 Self-adjoint extensions with induced potentials and the unitary scattering matrix

We need to check if by introducing the induced potentials, the self-adjoint extension will change as well. Similar analysis has been done in [16]. We still require for two states ψ and ϕ on a quantum graph G that the Hamiltonian is self-adjoint:

$$\langle \psi, H\phi\rangle = \langle H\psi, \phi\rangle, \quad \forall \psi, \phi \in \mathcal{H}_G \tag{3.31}$$

with again

$$\mathcal{H}_G = \bigoplus_{i=1}^{N} L^2([0,\infty[), \tag{3.32}$$

but now with the Hamiltonian on edge E_i is given by (3.13). We find, by partial integration that

$$\langle \psi, H\phi\rangle = \sum_{i=1}^{N}\int_0^\infty \mathrm{d}x\ \psi_i^*(x)\left(\frac{-\partial_x^2}{2m} + u_i\right)\phi_i(x) \tag{3.33}$$

$$= \frac{1}{2m}\sum_{i=1}^{N}\left[\psi_i^*(0)\partial_x\phi_i(0) - \partial_x\psi_i^*(0)\phi_i(0)\right] + \langle H\psi, \phi\rangle \tag{3.34}$$

so

$$\sum_{i=1}^{N}\psi_i^*(0)\partial_x\phi_i(0) = \sum_{i=1}^{N}\partial_x\psi_i^*\ (0)\phi_i(0), \tag{3.35}$$

which is an equivalent condition to the case with no induced potentials in section 2.2. By introducing the induced potentials, the BCs required for self-adjointness does not change, hence the results from [10] still hold, and thus the three requirements for the vertex remain:

$$A\psi(0)+B\psi'(0) = 0, \tag{3.36a}$$

$$AB^\dagger = BA^\dagger, \tag{3.36b}$$

$$\text{the composite } N \times 2N \text{ matrix } (A, B) \text{ has maximal rank } N. \tag{3.36c}$$

The components of $\psi(x)$ will now look like

$$\psi_b(x) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\varepsilon}{\sqrt{2\pi}} \sum_{a\in\mathcal{O}(\varepsilon)} c_a(\varepsilon)\chi_{ab}(x,\varepsilon), \tag{3.37}$$

with $c_a(\varepsilon)$ again being an annihilation operator, whose details will get discussed in section 5.2. So from (3.36a) we get by the same argumentation as in section 2.2

$$\sum_{j=1}^{N} \left(A_{bj}\chi_{aj}(0,\varepsilon) + B_{bj}\partial_x\chi_{aj}(x,\varepsilon)|_{x=0}\right) = 0, \quad a \in [1,n],\ b \in [1,N] \tag{3.38}$$

with the wavefunctions χ_{ab} given by (3.23).

$$\sum_{j=1}^{N} \left(A_{bj}S_{ja} + A_{bj}\delta_{aj} - iB_{bj}k_a^o\delta_{aj} + iB_{bj}k_j^oS_{ja} - B_{bj}k_j^cS_{ja}\right) = 0, \quad a \in [1,n],\ b \in [1,N] \tag{3.39}$$

leading to the matrix equation

$$S(\varepsilon) = -\left(A + iB\boldsymbol{k}\right)^{-1}\left(A - iB\boldsymbol{k}\right)\Pi_o^\top \tag{3.40}$$

with $\boldsymbol{k}$ given in (3.22), and $\Pi_o^\top$ is the block-defined matrix

$$\Pi_o^\top = \left(\begin{array}{c} \mathbf{1}_n \\ \hline \mathbf{0}_{(N-n)\times n} \end{array}\right) \quad \text{being } N \times n, \tag{3.41}$$

with $^\top$ denoting the transpose, $\mathbf{1}_n$ is the $n \times n$ identity matrix and $\mathbf{0}_{ab}$ is a $a \times b$ matrix filled with zeros. This makes the new scattering matrix $S(\varepsilon)$ have dimension $N \times n$. One could also have defined $\Pi_o^\top$ as an $N \times N$ projection matrix: with an $n \times n$ identity matrix in the top left corner as

$$\begin{pmatrix} \mathbf{1}_n & \mathbf{0}_{n\times\eta} \\ \mathbf{0}_{\eta\times n} & \mathbf{0}_{\eta\times\eta} \end{pmatrix}. \tag{3.42}$$

The scattering amplitude for closed channels would then be zero, instead of being undefined as with (3.41).

The Π's satisfy

$$P_o = \Pi_o^\top\Pi_o = \begin{pmatrix} \mathbf{1}_n & \mathbf{0}_{n\times\eta} \\ \mathbf{0}_{\eta\times n} & \mathbf{0}_{\eta\times\eta} \end{pmatrix}, \tag{3.43a}$$

$$\Pi_o\Pi_o^\top = \mathbf{1}_n \tag{3.43b}$$

and we define the invertible $n \times n$ matrices $\boldsymbol{\nu}^o$ and $\boldsymbol{\kappa}^o$ by

$$\boldsymbol{v}^o = \Pi_o^\top \boldsymbol{\nu}^o \Pi_o, \quad \boldsymbol{k}^o = \Pi_o^\top \boldsymbol{\kappa}^o \Pi_o \tag{3.44a}$$

$$\boldsymbol{\nu}^o = \Pi_o \boldsymbol{v}^o \Pi_o^\top, \quad \boldsymbol{\kappa}^o = \Pi_o \boldsymbol{k}^o \Pi_o^\top, \tag{3.44b}$$

Now $\boldsymbol{\nu}^o$ is the truncated $\boldsymbol{v}^o$ with m zeroes removed on both dimensions, meaning it is $n \times n$ with only non-zero components on the diagonal. When calculating the orthogonality (3.25), one ends up requiring the following construction of the scattering matrix to be unitary:

$$\hat{S}(\varepsilon) = \sqrt{\boldsymbol{\kappa}^o} \Pi_o S(\varepsilon) \sqrt{\boldsymbol{\kappa}^o}^{-1}, \tag{3.45}$$

that is now $n \times n$. A very similar construction has been considered in [18]. With the non-unitary part $S(\varepsilon)$ given by (3.40). Unitarity of the scattering matrix $\hat{S}$ is proven in Appendix D. In the case of all open channels $\varepsilon > u_N$, the above simplifies to

$$\hat{S}(\varepsilon) = \sqrt{\boldsymbol{k}} S(\varepsilon) \sqrt{\boldsymbol{k}}^{-1} = -\left(A\sqrt{\boldsymbol{k}}^{-1} + iB\sqrt{\boldsymbol{k}}\right)^{-1} \left(A\sqrt{\boldsymbol{k}}^{-1} - iB\sqrt{\boldsymbol{k}}\right). \tag{3.46}$$

And the existence of the inverse in this case is proven in Appendix A.

As alluded to earlier, $\boldsymbol{\kappa}^o(\varepsilon)$ is not invertible if it is evaluated at any of the induced potentials. Then it is the case that $\kappa^o(u_b)$, for any $b \in [1, N]$, is $b \times b$ with its very last entry $\kappa_b^o = 0$. Specifically for $a, b \in \mathcal{O}(\varepsilon)$ we find that

$$\hat{S}_{ab}(\varepsilon) = \left(\frac{\varepsilon - u_a}{\varepsilon - u_b}\right)^{1/4} S_{ab}(\varepsilon). \tag{3.47}$$

Based on numerical simulations, one concludes that for diagonal elements

$$\lim_{\varepsilon \to u_b^+} \hat{S}_{bb}(\varepsilon) = -1, \tag{3.48}$$

but we cannot conclude anything about non-diagonal elements, except

$$\lim_{\varepsilon \to u_b^+} |\hat{S}_{ab}(\varepsilon)|^2 = \delta_{ab}. \tag{3.49}$$

This hints at that channel b indeed is closed when the energy of the electron is exactly at the induced potential u_b, as indicated in the definition of a closed channel in (3.8). The channel opens as $\varepsilon > u_b$.

3.3 Conservation laws in first quantisation

At this point we can make several sanity checks, e.g. Kirchhoff's law and the continuity equation. We will show that the wavefunctions defined earlier satisfy Kirchhoff's law – specifically that the current is conserved. The construction below will also be used when calculating the current in second quantisation in section 5. The current is defined as

$$J_{ab}(x, \varepsilon) = \frac{1}{2im} \chi_{ab}^*(x, \varepsilon) \mathcal{R} \chi_{ab}(x, \varepsilon) \tag{3.50}$$

with

$$\chi_{ab}(x,\varepsilon) = \sqrt{v_a^o}^{-1}\left(e^{-ik_a^o x}\delta_{ab} + e^{i(k_b^o+ik_b^c)x}S_{ba}(\varepsilon)\right), \quad x\in(0,\infty),\ 1\le a\le n,\ 1\le b\le N. \tag{3.51}$$

Kirchoff's law states that the sum over each lead of currents has to vanish, hence we want to show that

$$\sum_{b=1}^{N} J_{ab}(x,\varepsilon) = 0, \quad \forall a\in\mathcal{O}(\varepsilon) \tag{3.52}$$

This is easily satisfied if all channels are open, meaning S is unitary and the momentum in each lead is conserved. However, we now will look at the situation with a general number $n\le N$ of open channels.

$$\begin{aligned}\chi_{ab}^*(x,\varepsilon)\mathcal{R}\chi_{ab}(x,\varepsilon) = \frac{1}{v_a^o}\Big[&-2ik_a^o\delta_{ab}^2 + i\delta_{ab}S_{ba}(\varepsilon)\left((k_b^o+ik_b^c)e^{ik_a^o x}e^{i(k_b^o+k_b^c)x} - k_a^o e^{ik_a^o x}e^{i(k_b^o+ik_b^c)x}\right)\\ &- i\delta_{ab}S_{ba}^*(\varepsilon)\left(k_a^o e^{-ik_a^o x}e^{-i(k_b^o-ik_b^c)x} - (k_b^o-ik_b^c)e^{-ik_a^o x}e^{-i(k_b^o-ik_b^c)x}\right) + 2ie^{-2k_b^c x}k_b^o|S_{ba}(\varepsilon)|^2\Big]\end{aligned} \tag{3.53}$$

So

$$\sum_{b=1}^{N} J_{ab}(x,\varepsilon) = \frac{-i}{2m}\frac{1}{v_a^o}\left[-2ik_a^o + 2i\sum_{b=1}^{N} e^{-2k_b^c}k_b^o|S_{ba}(\varepsilon)|^2\right] \tag{3.54a}$$

$$= -1 + \sum_{b=1}^{n} k_b^o|S_{ba}(\varepsilon)|^2(k_a^o)^{-1} \tag{3.54b}$$

$$= -1 + \sum_{b=1}^{n} |\hat{S}_{ba}(\varepsilon)|^2 \tag{3.54c}$$

$$= 0 \tag{3.54d}$$

where we used the unitarity of $\hat{S}$, and the transformation rule

$$|S_{ba}(\varepsilon)|^2 k_b^o = |\hat{S}_{ba}(\varepsilon)|^2 k_a^o, \quad b,a\in\mathcal{O}(\varepsilon) \tag{3.55}$$

applies, since both indices a and b, in (3.54b), indeed belong to open channels.

The continuity equation $\partial_t\rho(x,t) + \partial_x J_{ab}(x,t) = 0$, is satisfied since the density ρ does not depend on time, and $\partial_x[\chi_{ab}^*(x,\varepsilon)\mathcal{R}\chi_{ab}(x,\varepsilon)] = 0$, where terms not proportional to δ_{ba}, in (3.53), vanish, and the two terms proportional to S_{ba}^* and S_{ba} cancel independently.

3.4 The leads connect to thermal reservoirs

We now connect each lead to a reservoir R_i infinitely far away, which is parameterised by an inverse temperature $\beta_i = 1/T_i$ and a chemical potential μ_i. All the reservoirs we consider have $\mu_i > u_i$, such that electrons from the reservoir tunnel to the lead. The leads are in equilibrium with its corresponding reservoir.

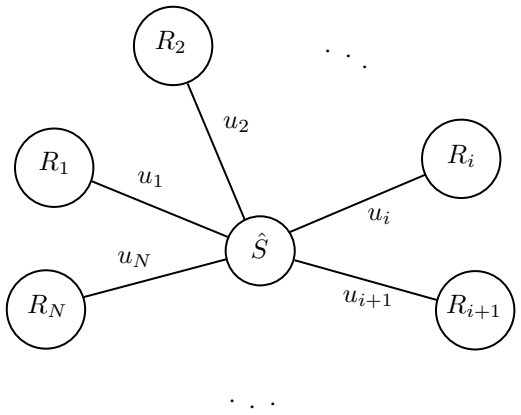


Figure 6: The graph G with each edge induced with a potential u and is connected to a reservoir R_i with inverse temperature β_i and chemical potential μ_i. The point-like scatterer is located at the vertex and is symbolised by the unitary scattering matrix $\hat{S}$.

The equilibrium regime is if all reservoirs are equal, meaning both temperature and chemical potentials are equal. We assume that every reservoir is filled according to a Fermi-Dirac distribution

$$f_j(\varepsilon - \mu_j) = \frac{1}{1 + e^{\beta_j(\varepsilon - \mu_j)}}, \tag{3.56}$$

and thus if $f_j = f_i$ for all i, j we are in equilibrium. The reservoirs R_i are modelled as infinitely large thermal baths, and they supply electrons to the leads such that all states are filled up to energy μ_i, at zero temperature. An incident electron on the reservoir, thus coming from the junction, is absorbed and thermalised with the reservoir. We also neglect interference between channels within each lead.

With the formalism in place, we will look at two examples of the BC matrices and calculate the scattering matrix in those cases.

4 Examples of the scattering matrix

We will now calculate the scattering matrix for some simple examples of BC matrices A and B. First we consider the Robin mixed boundary conditions. This is a linear combination of the two well-known boundary conditions: Dirichlet BC and Neumann BC. The former states only what values the wavefunction takes on the boundary, and the latter states what the derivative is on the boundary.

4.1 Robin mixed boundary conditions

The $N \times n$ scattering matrix is given by

$$S(\varepsilon) = -\left(A + iB\boldsymbol{k}\right)^{-1}\left(A - iB\boldsymbol{k}\right)\Pi_o^\top. \tag{4.1}$$

The unitary scattering matrix is

$$\hat{S}(\varepsilon) = \sqrt{\boldsymbol{\kappa}^o}\Pi_o S(\varepsilon)\sqrt{\boldsymbol{\kappa}^o}^{-1}. \tag{4.2}$$

The Robin BCs are given by

$$A = \begin{pmatrix} 1 & -1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & -1 \\ 0 & 0 & 0 & \cdots & 0 & -\alpha \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 1 & 1 & 1 & \cdots & 1 & 1 \end{pmatrix} \tag{4.3}$$

with a general proportionality constant $\alpha \in \mathbb{C}$. This means

$$\psi_1(0) = \psi_2(0) = \cdots = \psi_N(0), \quad \sum_{i=1}^{N} \partial_x \psi_i(0) = \alpha \psi_1(0). \tag{4.4}$$

$$A + iB\boldsymbol{k} = \begin{pmatrix} 1 & -1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & -1 \\ ik_1 & ik_2 & ik_3 & \cdots & ik_{N-1} & -\alpha + ik_N \end{pmatrix}. \tag{4.5}$$

By letting

$$\Sigma_{ab} = \sum_{j=a}^{b} k_j \tag{4.6}$$

for $b < N$ and

$$\Sigma_{aN} = \sum_{j=a}^{N} k_j + i\alpha \tag{4.7}$$

for $b = N$, where in particular

$$\Sigma_{1N} = \sum_{j=1}^{N} k_j + i\alpha, \tag{4.8}$$

we find

$$(A + iB\boldsymbol{k})^{-1} = \frac{1}{\Sigma_{1N}} \begin{pmatrix} \Sigma_{2N} & \Sigma_{3N} & \Sigma_{4N} & \Sigma_{5N} & \cdots & \Sigma_{NN} & i \\ -\Sigma_{11} & \Sigma_{3N} & \Sigma_{4N} & \Sigma_{5N} & \cdots & \Sigma_{NN} & i \\ -\Sigma_{11} & -\Sigma_{12} & \Sigma_{4N} & \Sigma_{5N} & \cdots & \Sigma_{NN} & i \\ -\Sigma_{11} & -\Sigma_{12} & -\Sigma_{13} & \Sigma_{5N} & \cdots & \Sigma_{NN} & i \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -\Sigma_{11} & -\Sigma_{12} & -\Sigma_{13} & -\Sigma_{14} & \cdots & \Sigma_{NN} & i \\ -\Sigma_{11} & -\Sigma_{12} & -\Sigma_{13} & -\Sigma_{14} & \cdots & -\Sigma_{1,N-1} & i \end{pmatrix} \tag{4.9}$$

This makes

$$S(\varepsilon) = -(A + iB\boldsymbol{k})^{-1}(A - iB\boldsymbol{k})\Pi_o^\top = -\frac{2}{\Sigma_{1N}} \begin{pmatrix} k_1 & \cdots & k_n \\ \vdots & \ddots & \vdots \\ k_1 & \cdots & k_n \end{pmatrix} - \Pi_o^\top \tag{4.10}$$

Now, to find the unitary scattering matrix:

$$\hat{S}(\varepsilon) = -\sqrt{\boldsymbol{\kappa}^o}\Pi_o(A+iBk)^{-1}(A-iBk)\Pi_o^\top\sqrt{\boldsymbol{\kappa}^o}^{-1} = -\frac{2}{\Sigma_{1N}}\sqrt{\boldsymbol{\kappa}^o}\begin{pmatrix} k_1 & \cdots & k_n \\ \vdots & \ddots & \vdots \\ k_1 & \cdots & k_n \end{pmatrix}\sqrt{\boldsymbol{\kappa}^o}^{-1} - \mathbf{1}_n \quad (4.11)$$

$$= -\frac{2}{\Sigma_{1N}}\begin{pmatrix} k_1 & \sqrt{k_1k_2} & \sqrt{k_1k_3} & \cdots & \sqrt{k_1k_n} \\ \sqrt{k_1k_2} & k_2 & \sqrt{k_2k_3} & \cdots & \sqrt{k_2k_n} \\ \sqrt{k_1k_3} & \sqrt{k_2k_3} & k_3 & \cdots & \sqrt{k_3k_n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \sqrt{k_1k_n} & \sqrt{k_2k_n} & \sqrt{k_3k_n} & \cdots & k_n \end{pmatrix} - \mathbf{1}_n. \quad (4.12)$$

Let

$$\Lambda = \begin{pmatrix} k_1 & \sqrt{k_1k_2} & \sqrt{k_1k_3} & \cdots & \sqrt{k_1k_n} \\ \sqrt{k_1k_2} & k_2 & \sqrt{k_2k_3} & \cdots & \sqrt{k_2k_n} \\ \sqrt{k_1k_3} & \sqrt{k_2k_3} & k_3 & \cdots & \sqrt{k_3k_n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \sqrt{k_1k_n} & \sqrt{k_2k_n} & \sqrt{k_3k_n} & \cdots & k_n \end{pmatrix} \quad (4.13)$$

then assuming for simplicity $\alpha \in \mathbb{R}$,

$$\hat{S}(\varepsilon) = \frac{2\sum_{j\in\mathcal{O}} k_j^o}{\left(\sum_{j\in\mathcal{O}} k_j^o\right)^2 + \left(\sum_{j\in\mathcal{C}} k_j^c + \alpha\right)^2}\Lambda - \mathbf{1}_n - \frac{2i\left(\sum_{j\in\mathcal{C}} k_j^c + \alpha\right)}{\left(\sum_{j\in\mathcal{O}} k_j^o\right)^2 + \left(\sum_{j\in\mathcal{C}} k_j^c + \alpha\right)^2}\Lambda \quad (4.14)$$

and by letting

$$K_{o/c} = \sum_{j\in\mathcal{O}/\mathcal{C}} k_j^{o/c} \geq 0, \quad \lambda_\alpha^2 = K_o^2 + (K_c+\alpha)^2 \quad (4.15)$$

then

$$\hat{S}(\varepsilon,\alpha) = 2\frac{K_o}{\lambda_\alpha^2}\Lambda - \mathbf{1}_n - 2i\frac{K_c+\alpha}{\lambda_\alpha^2}\Lambda \quad (4.16)$$

whose phase θ_{ab}, in polar coordinates, is

$$\theta_{ab}(\varepsilon,\alpha) = -\tan^{-1}\frac{K_c+\alpha}{K_o - \lambda_\alpha^2\delta_{ab}/2k_a}, \quad (4.17)$$

and since $\tan^{-1}x$ is a strictly increasing function it makes sense to take limits as $\alpha \to \pm\infty$:

$$\lim_{\alpha\to\pm\infty}\theta_{a\neq b}(\varepsilon,\alpha) = \mp\pi/2 \quad (4.18)$$

$$\lim_{\alpha\to\pm\infty}\theta_{a=b}(\varepsilon,\alpha) = 0 \quad (4.19)$$

One can also check numerically that $\theta_{a=b}(\varepsilon,\alpha) < 0$ for $\alpha \in \mathbb{R}$ and $\theta_{a\neq a}(\varepsilon,\alpha) > 0$. For a given finite interval of α and a constant ε, $\hat{S}_{ab}(\alpha)$ takes the shape of an ellipse arc in the complex plane, closing around

$$\lim_{\alpha\to\pm\infty}\hat{S}_{ab}(\varepsilon,\alpha) = -\delta_{ab}, \quad (4.20)$$

which reproduces the Dirichlet boundary conditions.

Setting $\alpha = 0$ gives a generalisation of the Neumann boundary conditions [5], and the unitary scattering matrix is

$$\hat{S}_{ab}(\varepsilon, 0) = 2\frac{K_o - iK_c}{K_o^2 + K_c^2}\Lambda - \mathbf{1}_n. \tag{4.21}$$

Further, by setting all induced potentials $\boldsymbol{u} = 0$, we find that the scattering matrix turns independent of energy. Scattering matrices that happen to be independent of energy, are of special interest since they correspond to critical points in statistical mechanics. However systems with non-zero induced potentials in the leads, may not be able to host energy-independent scattering matrices. The case of energy-independent scattering matrices without induced potentials has been explored fully in [10]. Now

$$\hat{S}(\varepsilon, \alpha = 0, \boldsymbol{u} = 0) = \frac{2}{N}\begin{pmatrix} 1 & \cdots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \end{pmatrix} - \begin{pmatrix} 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{pmatrix} \tag{4.22}$$

$$= \begin{pmatrix} \frac{2}{N} - 1 & \cdots & \frac{2}{N} \\ \vdots & \ddots & \vdots \\ \frac{2}{N} & \cdots & \frac{2}{N} - 1 \end{pmatrix}. \tag{4.23}$$

We will use examples for energy-independent scattering matrices in calculating the electric current and particle density in section 5.

4.2 A δ function potential

We will now look at the simplest example by letting A and B be diagonal. The resulting scattering matrix is also diagonal, and hence constitutes a family of systems in which there is no exchange of particles between leads or even channels, i.e. all incoming electron waves will exclusively get reflected. Using the fact that A and B are diagonal together with (3.23) and (3.38), we get that

$$S_{ba}(\varepsilon) = \frac{iB_{bb}k_a^o - A_{bb}}{A_{bb} + iB_{bb}k_b}\,\delta_{ba} \tag{4.24}$$

in which

$$S_{ba}(\varepsilon) = 0, \quad \forall a, \quad b > n(\varepsilon). \tag{4.25}$$

This can be interpreted as each (open) channel only interacts with itself, and closed channels interacts with nothing, so $k^c = 0$.

$$\hat{S}(\varepsilon) = -\Pi_o \left(A + iB\boldsymbol{k}^o\right)^{-1} \left(A - iB\boldsymbol{k}^o\right) \Pi_o^\top \tag{4.26}$$

is $n \times n$ and diagonal. The usual transformation $\sqrt{\boldsymbol{\kappa}^o} \cdots \sqrt{\boldsymbol{\kappa}^o}^{-1}$ cancels.

Since $\hat{S}$ is diagonal, and to be unitary, it can be written as

$$\hat{S}(\varepsilon) = e^{-i\theta(\varepsilon)}, \tag{4.27}$$

with $\theta(\varepsilon)$ being a diagonal, hermitian, complex $n \times n$ matrix. Let's rewrite $\hat{S}$

$$\hat{S}(\varepsilon) = -\Pi_o \left(A + iB\boldsymbol{k}^o\right)^{-1} \left(A - iB\boldsymbol{k}^o\right) \Pi_o^\top \tag{4.28a}$$

$$= -\Pi_o \left(A + iBP_o\boldsymbol{k}^o\right)^{-1} \left(A - iBP_o\boldsymbol{k}^o\right) P_o\Pi_o^\top \tag{4.28b}$$

$$= -\left[\Pi_o(A + iBP_o\boldsymbol{k}^o)\Pi_o^\top\right]^{-1} \Pi_o(A - iBP_o\boldsymbol{k}^o)\Pi_o^\top \tag{4.28c}$$

$$= -\left(\Pi_o A\Pi_o^\top + i\Pi_o B\Pi_o^\top \Pi_o\boldsymbol{k}^o\Pi_o^\top\right)^{-1} \left(\Pi_o A\Pi_o^\top - i\Pi_o B\Pi_o^\top \Pi_o\boldsymbol{k}^o\Pi_o^\top\right). \tag{4.28d}$$

We have used that $\boldsymbol{k}^o P_o = P_o\boldsymbol{k}^o = \boldsymbol{k}^o$, $P_o\Pi_o^\top = \Pi_o^\top$ and the fact that everything, with correct dimensions, commute. The rewriting $\Pi_o Z^{-1}\Pi_o^\top = [\Pi_o Z\Pi_o^\top]^{-1}$ obviously holds if Z is diagonal and invertible.

For convenience, we rename and rescale A, B and $\boldsymbol{k}^o$ as

$$\Pi_o A\Pi_o^\top \to A, \quad \Pi_o B\Pi_o^\top \to B, \quad \Pi_o\boldsymbol{k}^o\Pi_o^\top \to \boldsymbol{k}, \tag{4.29}$$

such that $\hat{S}$ can be rewritten in terms of

$$\hat{S}(\varepsilon) = -\left(A + iB\boldsymbol{k}\right)^{-1} \left(A - iB\boldsymbol{k}\right) = -\frac{AA^\dagger - 2i\boldsymbol{k}A^\dagger B - BB^\dagger\boldsymbol{k}^2}{AA^\dagger + BB^\dagger\boldsymbol{k}^2} = \cos\theta - i\sin\theta \tag{4.30}$$

The denominator is indeed invertible because of the rank condition $\operatorname{rank}((A, B)) = N$. By not considering the specific $\varepsilon = u_n$ then $\boldsymbol{k}$ is invertible and so the phase matrix is

$$\theta(\varepsilon) = \tan^{-1}\left(\frac{2AB^\dagger}{BB^\dagger\boldsymbol{k} - AA^\dagger\boldsymbol{k}^{-1}}\right), \tag{4.31}$$

since $AA^\dagger$, $BB^\dagger$, $AB^\dagger = (A^\dagger B)^\dagger = (AB^\dagger)^\dagger$ are real matrices. Arctangent with a diagonal matrix as argument is well-defined as the arctangent of each element. The explicit calculation for wavefunction orthogonality, with this specific scattering matrix, has been shown in Appendix E.

5 Field theory and observables

We will succinctly review the quantum field theory without induced potentials, as that will be used in conjunction with quenches in section 6. We will not calculate observables in this case, as that has been done in [5], [6]. Following this, we introduce the induced potentials, the fermionic fields and ground-states. In section 5.3 we calculate observables.

5.1 Field theory without induced potentials

The Hamiltonian is given by

$$H^0 = \bigoplus_{j=1}^{N} \frac{-\partial_x^2}{2m} \tag{5.1}$$

and $m > 0$ with eigenvalue

$$\varepsilon = \frac{k^2}{2m}, \tag{5.2}$$

as discussed in section 2. Where k is the momentum of the incoming electron and m is its mass, and the momentum is conserved across the junction. The two basis from section 2.1 constitute an orthonormal basis, and the corresponding algebras are then

$$\mathcal{A}^{\text{in}} \quad \text{is generated by} \quad \{c_i(k), c_i^\dagger(k) \mid k < 0,\ i \in [1, N]\}, \tag{5.3a}$$

$$\mathcal{A}^{\text{out}} \quad \text{is generated by} \quad \{c_i(k), c_i^\dagger(k) \mid k > 0,\ i \in [1, N]\}. \tag{5.3b}$$

The unitary transformation from $\mathcal{A}^{\text{in}}$ to $\mathcal{A}^{\text{out}}$ is given by the scattering matrix. This can easily be seen as e.g. considering the unitary transformation $\chi_a \to S^\dagger \chi_a = \bar{\chi}_a$: with components

$$\bar{\chi}_{b'}(x,k) = \sum_a \chi_{ba}(x,\varepsilon) S^\dagger_{ab'} = e^{-ikx} S^*_{b'b} + e^{ikx}\delta_{b'b} \tag{5.4}$$

The fields above form an anti-commuting algebra

$$\Big\{c_a(k_a), c_b(k_b)\Big\} = \Big\{c_a^\dagger(k_a), c_b^\dagger(k_b)\Big\} = 0, \quad \Big\{c_a(k_a), c_b^\dagger(k_b)\Big\} = 2\pi\delta_{ab}\delta(k_a - k_b). \tag{5.5}$$

The state, which one could take expectation values of, is $|\Omega(\boldsymbol{\beta}, \boldsymbol{\mu}, \boldsymbol{u} = 0)\rangle$ where index 0, indicates that there are no induced potentials $\boldsymbol{u} = 0$, where $\boldsymbol{\beta} = \{\beta_1, \cdots, \beta_N\}$ and $\boldsymbol{\mu} = \{\mu_1, \cdots, \mu_N\}$. Here each edge E_i for all $i = 1, ..., N$, is filled according to Fermi distributions $f_i(\varepsilon - \mu_i)$ in each edge E_i. At zero temperature each lead is filled from zero energy to μ, or in terms of momentum:

$$|\Omega(0, \mu, 0)\rangle = \prod_{i=1}^{N} \bigotimes_{0 \le k \le k_F} c_i^\dagger(k)\,|0\rangle \tag{5.6}$$

with $k_F = \sqrt{2m\mu}$. We will not calculate explicit observables, but explore the field theory and then include the potentials in the next section.

The above equation (5.5) does not hold if k_i and k_j have opposite sign. If the two momenta have opposite signs, then terms proportional to the scattering matrix must be added to the expectation value. The transformation between the negative and positive momentum basis is simply

$$c_i(k) = \sum_{j=1}^{N} S_{ij}(k) c_j(-k) \tag{5.7a}$$

$$c_i^\dagger(k) = \sum_{j=1}^{N} S_{ji}(-k) c_j^\dagger(-k). \tag{5.7b}$$

Of course if the system is in equilibrium, i.e. with a global chemical potential μ and inverse temperature β, the state $|\Omega(\beta, \mu, \boldsymbol{u})\rangle$, admits only equal Fermi-distributions $f_i = f_j$ at the reservoirs. The equilibrium and non-equilibrium situation of quantum star graphs with no induced potentials, have been studied in e.g. [5] and [6], respectively.

For both momenta positive or negative it is in general true that

$$\langle c_i^\dagger(k_i) c_j(k_j)\rangle = 2\pi\delta_{ij}\delta(k_i - k_j) f_i(\varepsilon(k) - \mu_i) \tag{5.8}$$

Now one can calculate physical observables, such as particle density, electric current, and conductance. This has been done in the aforementioned papers [5], [6]. We now turn on the potentials in the leads. This makes the field theory unlike the one just discussed.

5.2 Field theory with induced potentials

Now we turn on the induced potentials. The eigenenergy of state $|\chi_a(\varepsilon)\rangle$ is ε as

$$H\,|\chi_a(\varepsilon)\rangle = \varepsilon\,|\chi_a(\varepsilon)\rangle \tag{5.9}$$

for $a \in \mathcal{O}(\varepsilon)$ with

$$\mathcal{O}(\varepsilon) = \{j,\ \varepsilon - u_j > 0\}, \tag{5.10}$$

and as found in 3:

$$\varepsilon = \frac{k_i^2}{2m} + u_i \tag{5.11}$$

where u_i is the constant potential in edge E_i. The energy of the electron wave inserted in edge E_a with induced potential u_a, and momentum k_a has energy ε in all edges $i = 1, ..., N$. By assuming that $|\chi_a(\varepsilon)\rangle$ for $a \in \mathcal{O}(\varepsilon)$ form an orthonormal basis, the fermionic fields in position x and lead b are

$$\psi_b(x) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\varepsilon}{\sqrt{2\pi}} \sum_{a\in\mathcal{O}(\varepsilon)} c_a(\varepsilon)\chi_{ab}(x,\varepsilon), \quad x > 0 \tag{5.12a}$$

$$\psi_b^\dagger(x) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\varepsilon}{\sqrt{2\pi}} \sum_{a\in\mathcal{O}(\varepsilon)} c_a^\dagger(\varepsilon)\chi_{ab}^*(x,\varepsilon), \quad x > 0 \tag{5.12b}$$

The field $\psi(x) = (\psi_1(x), \cdots, \psi_N(x))^\top$ satisfy the BCs in (3.36a):

$$A\psi(0) + B\psi'(0) = 0. \tag{5.13}$$

For a star graph the combination x and b on $\psi_b(x)$ completely determines the position on the star graph, with $b = 1, ..., N$ and $x > 0$. The wavefunctions and scattering matrices in (5.12) are

$$\chi_{ab}(x,\varepsilon) = \sqrt{v_a^o}^{-1}\left(e^{-ik_a^o x}\delta_{ba} + e^{i(k_b^o + ik_b^c)x}S_{ba}(\varepsilon)\right), \tag{5.14}$$

where $\boldsymbol{k}$ is the diagonal, invertible and complex matrix

$$\boldsymbol{k} = \mathrm{diag}\left(\sqrt{2m(\varepsilon - u_1)}, ..., \sqrt{2m(\varepsilon - u_N)}\right) \tag{5.15}$$

and $\boldsymbol{k}^o = \mathrm{Re}\{\boldsymbol{k}\}$, and $\boldsymbol{k}^c = \mathrm{Im}\{\boldsymbol{k}\}$. The creation and annihilation operators $c^\dagger$ and c in (5.12), are defined through the anti-commutation relations

$$\left\{c_a(\varepsilon), c_b(\varepsilon')\right\} = \left\{c_a^\dagger(\varepsilon), c_b^\dagger(\varepsilon')\right\} = 0, \quad \left\{c_a(\varepsilon), c_b^\dagger(\varepsilon')\right\} = 2\pi\delta_{ab}\delta(\varepsilon - \varepsilon') \tag{5.16}$$

for $a \in \mathcal{O}(\varepsilon)$ and $b \in \mathcal{O}(\varepsilon')$. The fields above are set to have units $1/\sqrt{\mathrm{E}}$ and $\psi_b(x)$ then have $1/\sqrt{\mathrm{L}}$, since χ has $1/\sqrt{\mathrm{EL}}$. By assuming that the wavefunctions $\chi_{ab}(x,\varepsilon)$ form a complete set, meaning they satisfy

$$\mathcal{I}_{bb'} \equiv \int_{-\infty}^{\infty} \mathrm{d}\varepsilon \sum_{a\in\mathcal{O}(\varepsilon)} \chi_{ab'}^*(\varepsilon,x')\chi_{ab}(\varepsilon,x) = 2\pi\delta_{b'b}\delta(x'-x), \tag{5.17}$$

which means

$$\mathcal{I}_{bb'} = \int_{-\infty}^{\infty} \mathrm{d}\varepsilon \sum_{a\in\mathcal{O}(\varepsilon)} \frac{1}{v_a^o} \Big\{ e^{-ik_a^o x} e^{ik_a^o x'} \delta_{ba}\delta_{ab'} + e^{-ik_a^o x} e^{-i(k_{b'}^o - ik_{b'}^c)x'} S^*_{b'a}(\varepsilon)\delta_{ba} + \tag{5.18}$$

$$+ e^{ik_a^o x'} e^{i(k_b^o + ik_b^c)x} S_{ba}(\varepsilon)\delta_{b'a} + e^{i(k_b^o + i_b^c)x} e^{-i(k_{b'}^o - ik_{b'}^c)x'} S_{ba}(\varepsilon) S^*_{b'a}(\varepsilon) \Big\} \tag{5.19}$$

$$= \delta_{b'b} \int_{u_b}^{\infty} \mathrm{d}\varepsilon \frac{e^{ik_b^o(x'-x)}}{v_b^o} + \int_{-\infty}^{\infty} \mathrm{d}\varepsilon\ e^{i(k_b^o + i_b^c)x} e^{-i(k_{b'}^o - ik_{b'}^c)x'} \sum_{a\in\mathcal{O}(\varepsilon)} S_{ba}(\varepsilon) \sqrt{v_a^o}^{-1} \sqrt{v_a^o}^{-1} S^\dagger_{ab'}(\varepsilon) \tag{5.20}$$

$$+ \int_{u_b}^{\infty} \mathrm{d}\varepsilon \frac{e^{-ik_b^o x} e^{-i(k_{b'}^o - ik_{b'}^c)x'}}{v_b^o} S^\dagger_{bb'}(\varepsilon) + \int_{u_{b'}}^{\infty} \mathrm{d}\varepsilon \frac{e^{ik_{b'}^o x'} e^{i(k_b^o + ik_b^c)x}}{v_{b'}^o} S_{bb'}(\varepsilon) \tag{5.21}$$

$$= \delta_{b'b} \left(\pi\delta(x'-x) + \frac{i}{x'-x} \right) + L + Q_{bb'} + Q^\dagger_{bb'} \tag{5.22}$$

with

$$L = \int_{-\infty}^{\infty} \mathrm{d}\varepsilon\ e^{i(k_b^o + i_b^c)x} e^{-i(k_{b'}^o - ik_{b'}^c)x'} \sum_{a\in\mathcal{O}(\varepsilon)} S_{ba}(\varepsilon) \sqrt{v_a^o}^{-1} \sqrt{v_a^o}^{-1} S^\dagger_{ab'}(\varepsilon) \tag{5.23}$$

$$= \int_{\min(u_{b'},u_b)}^{\infty} \mathrm{d}\varepsilon\ e^{ik_b^o x} e^{-ik_{b'}^o x'} \sum_{a\in\mathcal{O}(\varepsilon)} \sqrt{v_b^o}^{-1} \sqrt{v_b^o} S_{ba} \sqrt{v_{b'}^o}^{-1} \sqrt{v_b^o}^{-1} S^\dagger_{ab'} \sqrt{v_{b'}^o} \sqrt{v_{b'}^o}^{-1} \tag{5.24}$$

$$+ \int_{-\infty}^{\min(u_b,u_{b'})} \mathrm{d}\varepsilon e^{-ik_b^c x} e^{-ik_{b'}^c x'} \sum_{a\in\mathcal{O}(\varepsilon)} S_{ba}(\varepsilon) \sqrt{v_a^o}^{-1} \sqrt{v_a^o}^{-1} S^\dagger_{ab'}(\varepsilon) \tag{5.25}$$

$$= \delta_{b'b} \int_{\min(u_{b'},u_b)}^{\infty} \mathrm{d}\varepsilon\ e^{-k_b^o(x'-x)} \frac{1}{v_b^o} + \int_{-\infty}^{\min(u_b,u_{b'})} \mathrm{d}\varepsilon e^{-ik_b^c x} e^{-ik_{b'}^c x'} \sum_{a\in\mathcal{O}(\varepsilon)} S_{ba}(\varepsilon) \sqrt{v_a^o}^{-1} \sqrt{v_a^o}^{-1} S^\dagger_{ab'}(\varepsilon) \tag{5.26}$$

$$= \delta_{b'b} \left(\pi\delta(x'-x) + \frac{i}{x'-x} \right) + \int_{-\infty}^{\min(u_b,u_{b'})} \mathrm{d}\varepsilon\ e^{-ik_b^c x} e^{-ik_{b'}^c x'} \sum_{a\in\mathcal{O}(\varepsilon)} S_{ba}(\varepsilon) \sqrt{v_a^o}^{-1} \sqrt{v_a^o}^{-1} S^\dagger_{ab'}(\varepsilon) \tag{5.27}$$

and

$$Q_{bb'} = \int_{u_b}^{\infty} \mathrm{d}\varepsilon \frac{e^{-ik_b^o x} e^{-i(k_{b'}^o - ik_{b'}^c)x'}}{v_b^o} S^\dagger_{bb'}(\varepsilon). \tag{5.28}$$

So we indeed see that

$$\mathcal{I}_{bb'} = 2\pi\delta_{bb'}\delta(x'-x) + 2i\delta_{b'b}/(x'-x) + Q_{bb'} + Q^\dagger_{bb'} + \int_{-\infty}^{\min(u_b,u_{b'})} \mathrm{d}\varepsilon\ e^{-ik_b^c x} e^{-ik_{b'}^c x'} \sum_{a\in\mathcal{O}(\varepsilon)} S_{ba}(\varepsilon) \sqrt{v_a^o}^{-1} \sqrt{v_a^o}^{-1} S^\dagger_{ab'}(\varepsilon) \tag{5.29}$$

we get the anti-commutation relations for $\psi_b(x)$ and $\psi_b^\dagger(x)$ are

$$\Big\{ \psi_a(x), \psi_b(x') \Big\} = \Big\{ \psi_a^\dagger(x), \psi_b^\dagger(x') \Big\} = 0, \quad \Big\{ \psi_a(x), \psi_b^\dagger(x') \Big\} = 2\pi\delta(x'-x)\delta_{ab}. \tag{5.30}$$

The completeness assumption above leads one to require that there are no bound states at the vertex. The existence of bound states at the vertex is explored in [19]. If we would include these bound states,

the fields $\psi_b(x)$ in (5.12) would need an additional term that is the contributions from the bound state at the vertex, and completeness would then be restored. With these commutation relations in hand, we will begin to define and calculate physical quantities, like the energy operator, particle current, particle density, and heat current, and we will find agreement in the limit $\boldsymbol{u} = 0$.

5.3 Observables

In this section, we will use the quantum field theory from the last section to explore the electronic transport properties of the quantum star graph with induced potentials. We will calculate the electric and heat current, particle density and differential conductance. The equilibrium and non-equilibrium case, has been studied by e.g. B. Bellazzini and M. Mintchev in [5] and [6] and in the following we extend the formalism to include induced potentials.

In one of the original papers by Landauer and Büttiker [3], the following was mentioned about the possibility of imaginary wavenumber: "*Evanescent states with imaginary value of the wave number parallel to the wire can be neglected. They cannot contribute to the current, and can only have an effect on the chemical potential right at the interface between the scatterer and the ideal conductor*". We will also find this to be the case, but these evanescent states do contribute to, e.g., the particle density. The particle density will gain an x-dependence which will get manifested as Friedel oscillations for scale invariant scattering matrices.

First, we define the observable as operators, and then calculate their corresponding expectation value. Lastly, we discuss some conservation laws and symmetries about the system.

The Hamiltonian is now

$$H = \int_0^\infty \mathrm{d}x \sum_{b=1}^{N} \left[\psi_b^\dagger(x) \frac{-\partial_{b,x}^2}{2m} \psi_b(x) + u_b \psi_b^\dagger(x) \psi_b(x) \right]. \tag{5.31}$$

By using (5.12), we can write it in the $\chi_a(\varepsilon)$ basis.

$$\begin{aligned} H = \int_0^\infty \mathrm{d}x \sum_{b=1}^{N} \iint_{-\infty}^{\infty} \frac{\mathrm{d}\varepsilon \mathrm{d}\varepsilon'}{2\pi} \sum_{\substack{a' \in \mathcal{O}(\varepsilon') \\ a \in \mathcal{O}(\varepsilon)}} \frac{c_{a'}^\dagger(\varepsilon') c_a(\varepsilon)}{\sqrt{v_{a'}^{o\prime} v_a^o}} \Bigg[\left(\frac{k_a^{o2}}{2m} + u_b \right) e^{i(k_{a'}^o - k_a^o)x} \delta_{a'b} \delta_{ab} \\ + \left(\frac{(k_b^o + ik_b^c)^2}{2m} + u_b \right) e^{ik_{a'}^{o\prime} x} e^{i(k_b^o + ik_b^c)x} \delta_{a'b} S_{ba}(\varepsilon) + \left(\frac{k_a^{o2}}{2m} + u_b \right) e^{-ik_a^o x} e^{-i(k_b^{o\prime} - ik_b^{c\prime})x} \delta_{ab} S_{ba}^*(\varepsilon') \\ + \left(\frac{(k_b^o + ik_b^c)^2}{2m} + u_b \right) e^{i(k_b^o + ik_b^c)x} e^{-i(k_b^{o\prime} - ik_b^{c\prime})x} S_{ba}(\varepsilon) S_{ba}^*(\varepsilon') \Bigg]. \end{aligned} \tag{5.32}$$

We can now perform the b sum, and find that all round brackets equal ε, since $k_a^{o2} = (k_a^o + ik_a^c)^2$ for $a \in \mathcal{O}$. We then immediately reintroduce the b sum with appropriate $\delta_{a'b}$ and δ_{ab}, and recognise the

four terms as $\sum_b \chi^*_{a'b}\chi_{ab}$. Thus

$$H = \int \mathrm{d}x \sum_b \iint \frac{\mathrm{d}\varepsilon\, \mathrm{d}\varepsilon'}{2\pi} \sum_{a'a} c^\dagger_{a'}(\varepsilon')c_a(\varepsilon)\varepsilon\chi^*_{a'b}(x,\varepsilon')\chi_{ab}(x,\varepsilon) \tag{5.33}$$

$$H = \int_0^\infty \mathrm{d}\varepsilon \sum_{a\in\mathcal{O}(\varepsilon)} c^\dagger_a(\varepsilon)c_a(\varepsilon)\varepsilon. \tag{5.34}$$

The time evolution of $\psi_b(x)$ is found by defining

$$\hat{n}_a(\varepsilon) = c^\dagger_a(\varepsilon)c_a(\varepsilon) \tag{5.35}$$

and quickly verify that

$$[c_a(\varepsilon), \hat{n}_{a'}(\varepsilon')] = 2\pi\delta_{aa'}\delta(\varepsilon'-\varepsilon)c_a(\varepsilon), \tag{5.36}$$

and by induction one finds for any $m \in \mathbb{N}$

$$\left[c_a(\varepsilon), (\hat{n}_{a'}(\varepsilon'))^m\right] = (2\pi\delta_{aa'}\delta(\varepsilon-\varepsilon'))^m\, c_a(\varepsilon) \tag{5.37}$$

such that

$$c_a(\varepsilon)e^{-iHt} = e^{-i\varepsilon t}e^{-iHt}c_a(\varepsilon). \tag{5.38}$$

The time evolution of the fields $\psi_b(x)$ and $\psi^\dagger_b(x)$ is then

$$\psi_b(x,t) = e^{iHt}\psi_b(x)e^{-iHt} \tag{5.39a}$$

$$= \int_{-\infty}^\infty \frac{\mathrm{d}\varepsilon}{\sqrt{2\pi}} \sum_{a\in\mathcal{O}(\varepsilon)} c_a(\varepsilon)\chi_{ab}(x,\varepsilon)e^{-i\varepsilon t} \tag{5.39b}$$

$$\psi^\dagger_b(x,t) = \int_{-\infty}^\infty \frac{\mathrm{d}\varepsilon}{\sqrt{2\pi}} \sum_{a\in\mathcal{O}(\varepsilon)} c^\dagger_a(\varepsilon)\chi^*_{ab}(x,\varepsilon)e^{i\varepsilon t}. \tag{5.39c}$$

The non-equilibrium state $|\Omega(\boldsymbol{\beta},\boldsymbol{\mu},\boldsymbol{u})\rangle$ with induced potentials, is the state with each edge E_i filled from u_i to μ_i. This is the state we take expectation values with respect to. At zero temperature this state is

$$|\Omega(\infty,\boldsymbol{\mu},\boldsymbol{u})\rangle = \prod_{i=1}^N \bigotimes_{u_i\le\varepsilon\le\mu_i} c^\dagger_i(\varepsilon)\,|0\rangle\,. \tag{5.40}$$

Any expectation value $\langle\cdot\rangle$ is now taken with respect to $\langle\Omega(\boldsymbol{\beta},\boldsymbol{\mu},\boldsymbol{u})|\cdot|\Omega(\boldsymbol{\beta},\boldsymbol{\mu},\boldsymbol{u})\rangle$, with the dot representing the operator whose expectation value we wish to calculate. At non-zero temperature, we say that

$$\langle c^\dagger_{a'}(\varepsilon')c_a(\varepsilon)\rangle = f_a(\varepsilon-\mu_a)\delta_{a'a}\delta(\varepsilon'-\varepsilon) \tag{5.41}$$

with $f_a(\varepsilon-\mu_a)$ the Fermi distribution function

$$f_a(\varepsilon-\mu_a) = \frac{1}{1+e^{\beta_a(\varepsilon-\mu_a)}}, \tag{5.42}$$

with $\beta_a = 1/T_a$ the inverse temperature associated with each reservoir R_a, as well as the chemical potential μ_a.

We begin by calculating the electric current in units of the elementary charge.

$$J_b(x,t) = \frac{i}{2m}\psi_b^\dagger(x,t)\mathcal{R}\psi_b(x,t) \tag{5.43}$$

with

$$\mathcal{R} = \vec{\partial}_x - \overleftarrow{\partial}_x, \tag{5.44}$$

the arrow indicating which direction the derivative is acting.

$$J_b(x,t) = \frac{i}{2m}\iint_0^\infty \frac{\mathrm{d}\varepsilon\ \mathrm{d}\varepsilon'}{2\pi} \sum_{\substack{a\in\mathcal{O}(\varepsilon)\\ a'\in\mathcal{O}(\varepsilon')}} c_{a'}^\dagger(\varepsilon')c_a(\varepsilon)\ \chi_{a'b}^*(x,\varepsilon')\mathcal{R}\chi_{ab}(x,\varepsilon)e^{i(\varepsilon'-\varepsilon)t}. \tag{5.45}$$

We calculate the expectation value of the current $J_b(x,t)$ with the reservoirs at non-zero temperatures as well as with induced leads, in the same state and find that the particle current I^{part} is

$$I_b^{\text{part}} = \langle J_b(x,t)\rangle \tag{5.46a}$$

$$= \frac{i}{2m}\iint_{-\infty}^\infty \frac{\mathrm{d}\varepsilon\ \mathrm{d}\varepsilon'}{2\pi} \sum_{\substack{a\in\mathcal{O}(\varepsilon)\\ a'\in\mathcal{O}(\varepsilon')}} \langle c_{a'}^\dagger(\varepsilon')c_a(\varepsilon)\rangle\ \chi_{a'b}^*(x,\varepsilon')\mathcal{R}\chi_{ab}(x,\varepsilon)e^{-i(\varepsilon-\varepsilon')t} \tag{5.46b}$$

$$I_b^{\text{part}} = \frac{1}{2\pi}\int_{u_b}^\infty \mathrm{d}\varepsilon \sum_{a\in\mathcal{O}(\varepsilon)} \left[f_b(\varepsilon) - f_a(\varepsilon)\right]|\hat{S}_{ba}(\varepsilon)|^2 \tag{5.46c}$$

$$I_b^{\text{part}} = \frac{1}{2\pi}\int_{u_b}^\infty \mathrm{d}\varepsilon \sum_{a\in\mathcal{O}(\varepsilon)} \left[\delta_{ba} - |\hat{S}_{ba}(\varepsilon)|^2\right] f_a(\varepsilon) \tag{5.46d}$$

Full derivation is in Appendix G. The b index on $\hat{S}$ can seem ambiguous, since the left hand side $b = 1, ..., N$, but on the right, specifically the index on $\hat{S}_{ba}$ is limited to $b = 1, ..., n(\varepsilon)$, but since we integrate over an ε-interval where $\varepsilon \geq u_b$, this makes b always open. This can also be seen as, for a given energy $\varepsilon_0 > u_b$ then $n(\varepsilon_0) \geq n(u_b) = b$. We remember that $k_b^o = \theta(\varepsilon - u_b)\sqrt{2m(\varepsilon - u_b)}$ and used

$$|S_{ba}(\varepsilon)|^2 k_b^o = |\hat{S}_{ba}(\varepsilon)|^2 k_a^o, \quad b, a \in \mathcal{O}(\varepsilon), \tag{5.47}$$

We also see that the current is both position and time independent. By nature of the continuity equation, we must have that the particle density cannot depend on time, in accordance with not accumulating charge along the edges. The system is thus in a non-equilibrium steady state. If there are no induced potentials:

$$I_b^{\text{part}}(u=0) = \frac{1}{2\pi}\int_0^\infty \mathrm{d}\varepsilon \sum_{a=1}^N \left[\delta_{ba} - |S_{ba}(\varepsilon)|^2\right] f_a(\varepsilon), \tag{5.48}$$

the momentum would be conserved, so converting to a k integral would leave us with the same equation for the current as [6] (without e being multiplied on), which indeed is reassuring. For zero temperature, the current is

$$I_b^{\text{part}}(\boldsymbol{\beta} = \infty) = \frac{1}{2\pi} \sum_{a|\mu_a > u_b} \int_{u_a}^{\mu_a} \mathrm{d}\varepsilon\ \theta(\varepsilon - u_b)\left[\delta_{ba} - |S_{ba}(\varepsilon,\alpha)|^2\right]. \tag{5.49}$$

We will now consider the BC's in section 4.1, i.e. the mixed Robin BC's, parameterised by α, so $I_b^{\text{part}}(\boldsymbol{\beta} = \infty, \alpha)$. We found that

$$\lim_{\alpha \to \pm\infty} \hat{S}_{ab}(\varepsilon, \alpha) = -\delta_{ab}. \tag{5.50}$$

The current $I_b^{\text{part}}(\boldsymbol{\beta} = 0, \alpha)$, i.e. the current, for all channels, should vanish as $\alpha \to \pm\infty$. The current as a function of α is shown on figure 7.

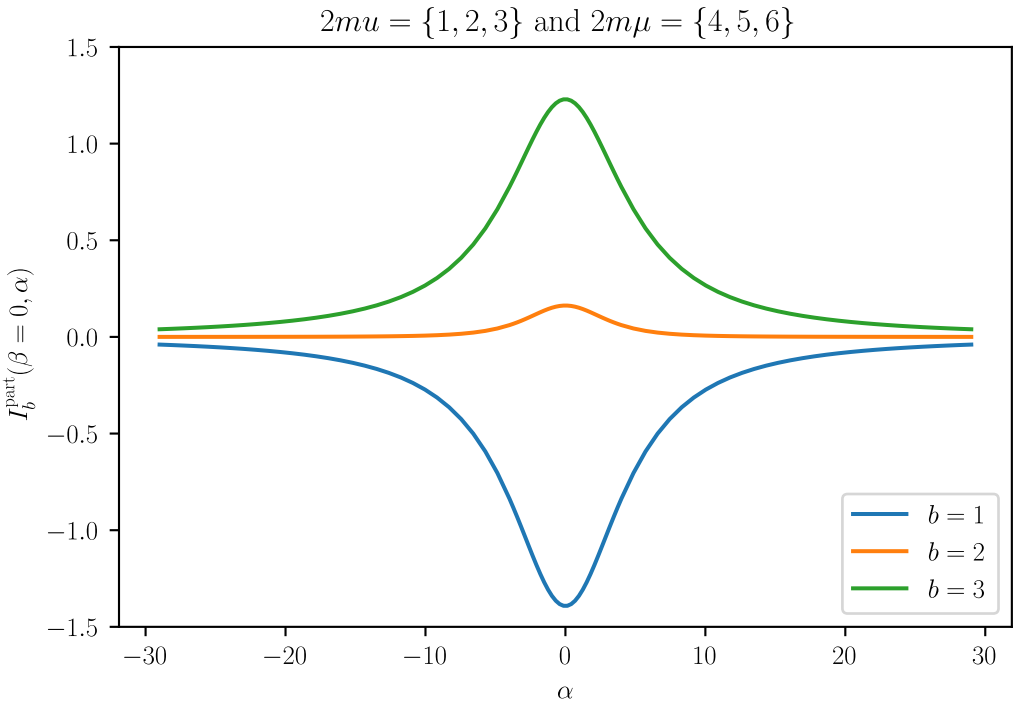


Figure 7: Here the b refers to the channel number in I_b. Channel 1 has $2mu_1 = 1$ and $2m\mu_1 = 4$, etc. The mass is set to $m = 1/2$. The BC matrices are given in (4.3).

The lead with lowest potential is more susceptible to electron flow, hence $b = 1$ has negative current. Of course, the total current flowing out of the junction has to vanish according to Kirchhoff. For a non-zero temperature:

$$\sum_{b=1}^{N} I_b^{\text{part}} = \frac{1}{2\pi} \int_0^\infty \mathrm{d}\varepsilon \sum_{a \in \mathcal{O}(\varepsilon)} \sum_{b \in \mathcal{O}(\varepsilon)} \left[\delta_{ba} - |\hat{S}_{ba}(\varepsilon)|^2 \right] f_a(\varepsilon) = 0. \tag{5.51}$$

We also conclude from (5.46c), that there will run no current if all Fermi-distributions are equal at the reservoirs. This is the case if all the temperatures β_i and the chemical potential are equal, which makes good sense. The current also vanishes if $\delta_{ba} = |\hat{S}_{ba}(\varepsilon)|^2$, which, e.g., is the case for the example for Robin B.C. discussed in section 4.1, where we set $\alpha \to \pm\infty$, and regained the Dirichlet B.C.: $\hat{S}_{ba} = \delta_{ba}$, or more generally $\hat{S}_{ba}(\varepsilon) = \delta_{ba} e^{i\phi_a(\varepsilon)}$, $\phi_a(\varepsilon) \in \mathbb{R}$. We can now find the electric current for

the scale invariant scattering matrix found in section 4.1. It is given by

$$S_{ba} = \frac{2}{N} - \delta_{ba}. \tag{5.52}$$

Here there is no induced leads. The current at zero temperature is simply

$$I_b^{\text{part}}(\boldsymbol{\beta} = \infty) = \sum_{a=1}^{N} \int_0^{\mu_a} \mathrm{d}\varepsilon \left(\frac{4}{N}\delta_{ba} - \frac{4}{N^2} \right) \tag{5.53}$$

$$= \frac{4}{N}\mu_b - \frac{4}{N^2} \sum_{a=1}^{N} \mu_a. \tag{5.54}$$

Another basic physical observable is the conductance G_{ab} where the indices a, b indicate from which channels the current is running to and from. We also reintroduce the charge e as $eI_b^{\text{part}} = I_b^{\text{ch}}$, with I_b^{ch} being in the charge current that defines the (differential) conductance as $G_{bb'} = \partial I_b^{\text{ch}}/\partial V_{b'}$ with $\mu_{b'} = eV_{b'}$. Here $V_{b'}$ is the voltage across reservoir $R_{b'}$. The conductance is then

$$G_{bb'}(\mu_{b'}) = e^2 \frac{\partial I_b^{\text{part}}}{\partial \mu_{b'}} = \frac{e^2}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}\varepsilon \; \theta(\varepsilon - u_b)\theta(\varepsilon - u_{b'}) \left[\delta_{bb'} - |\hat{S}_{bb'}(\varepsilon)|^2 \right] \frac{\partial f_{b'}(\varepsilon)}{\partial \mu_{b'}}. \tag{5.55}$$

This is the general formula. If the reservoirs are not filled according to a Fermi-Dirac distribution, then the following approximation at $T = 0$ does not hold. The conductance at zero temperature $G^0_{bb'}$, can be found by setting $f_a(\varepsilon - \mu) \to \theta(\mu - \varepsilon)$ and the derivative $\partial_\mu f_a(\varepsilon - \mu) \to +\delta(\varepsilon - \mu)$, we get

$$G^0_{bb'}(\mu_{b'}) = \frac{e^2}{2\pi} \theta(\mu_{b'} - u_b) \left(\delta_{bb'} - |\hat{S}_{bb'}(\mu_{b'})|^2 \right) \tag{5.56}$$

where we have assumed that $\mu_{b'} > u_{b'}$, since if this is not the case, no electrons are being transferred to the lead from reservoirs (at zero temperature). Due to unitarity of $\hat{S}$, $|\hat{S}_{bb'}(\mu_{b'})|^2 \leq 1$, so $-1 \leq G^0_{bb'}/e^2 \leq 1$. From above (5.56), the conductance is negative for all $b' \neq b$ and positive for diagonal elements (or zero if everything is reflected). The graph of the conductance at zero temperature G^0 is shown on figure 8 for $N = 3$ and with induced potentials given by $2mu = 2m\{u_1, u_2, u_3\} = \{1, 2, 3\}$, and BCs given by the Robin BCs i.e. that

$$\psi_1(0) = \cdots = \psi_N(0), \quad \psi_1'(0) + \cdots + \psi_N'(0) = \alpha\psi_1(0). \tag{5.57}$$

Notice this BC is symmetric under any edge permutations. This is of course, not a universal feature, as one could exchange a 0 in the B matrix in (4.3) to a 1 and this symmetry would be broken.

The conductance is of course only defined for values of $\mu_{b'} > u_{b'}$, else it must be zero, which is illustrated below by the fact that each subgraph is not defined as $\mu_{b'} < u_{b'}$. Let's focus on panel a) on figure 8. As $1 < 2m\mu_1 < 2$, a current can only get reflected in edge 1, as the induced potentials at the others are > 2, i.e. closed channels. As $2 < 2m\mu_1 < 3$, a current can flow from edge 1 to 2 (orange graph), but still get reflected (blue), and no current goes from $b = 1$ to $b = 3$ as edge $b = 3$ is still closed. As $\mu_1 > 3$ a current from $b' = 1$ can flow to all three channels. And by the same token, on b) current can flow immediately in $b = 1$ and $b = 2$, but only to $b = 3$ after $\mu_2 > u_3$. Since μ_3 is the largest chemical potential, in c) are other channels open.

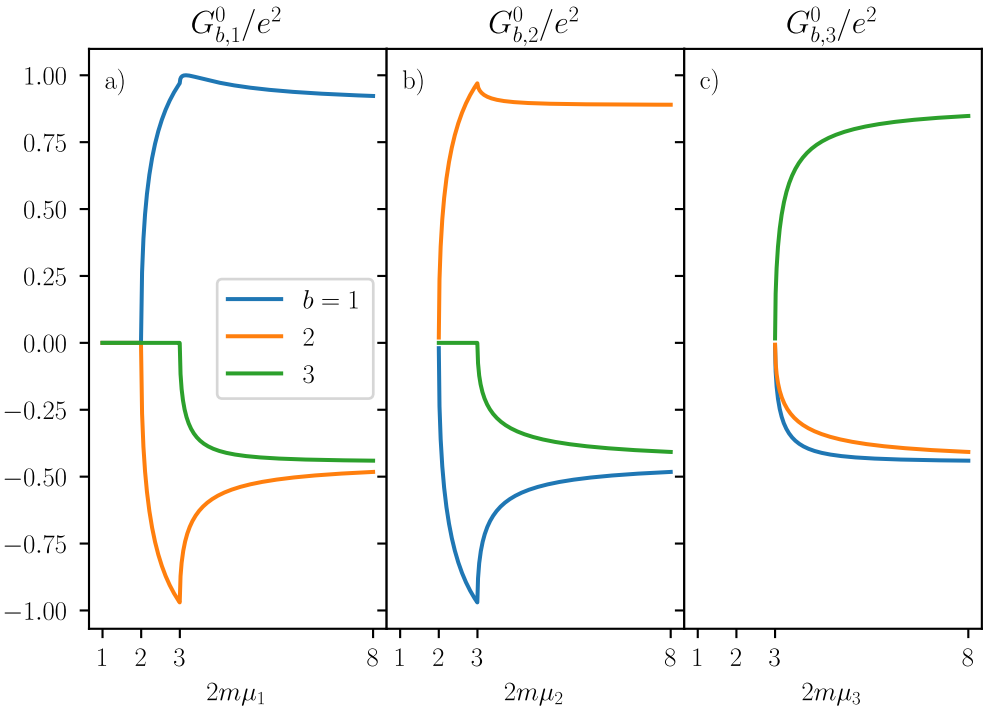


Figure 8: The conductance at zero temperature is shown, given by (5.56) for $N = 3$ channels. The induced potentials in this case are $2mu = 2m\{u_1, u_2, u_3\} = \{1, 2, 3\}$, given in arbitrary units of p^2, where p is momentum. The B.C. matrices A and B are given by the Robin B.C.s (4.3), with $\alpha = 0$, and we have set $m = 1/2$. Panel a), b) and c) show the conductance from channel $b' = 1$, $b' = 2$ and $b' = 3$, to all 3 channels respectively. Kirchhoff's law also look to hold, by inspecting that the sum of the three graphs for each sub-figure, vanish.

A similar graph for $2mu = \{1, 2, 2\}$, is on figure 11 in Appendix F. The influence of α can be seen on figure 12 and 13. The general feature is that as $\alpha \to \infty$ the conductance vanishes, i.e. each lead becomes isolated. This is in agreement with (4.20) stating that $\lim_{\alpha\to\infty} \hat{S}_{ab}(\varepsilon, \alpha) = -\delta_{ab}$.

Next up is the particle density ρ. The particle density operator is

$$\rho_b(x) = \psi_b^\dagger(x)\psi_b(x), \tag{5.58}$$

and the expectation value is then

$$\langle \rho_b(x) \rangle = \iint \frac{\mathrm{d}\varepsilon\, \mathrm{d}\varepsilon'}{2\pi} \sum_{a',a} \langle c_{a'}^\dagger(\varepsilon') c_a(\varepsilon) \rangle \chi^*_{a'b}(x, \varepsilon') \chi_{ab}(x, \varepsilon) \tag{5.59}$$

$$= \int_{u_b}^{\infty} \frac{\mathrm{d}\varepsilon}{2\pi} \sum_{a \in \mathcal{O}(\varepsilon)} f_a(\varepsilon - \mu_a) |\chi_{ab}(x, \varepsilon)|^2 + \int_{-\infty}^{u_b} \frac{\mathrm{d}\varepsilon}{2\pi} \sum_{a \in \mathcal{O}(\varepsilon)} f_a(\varepsilon - \mu_a) |\chi_{ab}(x, \varepsilon)|^2 \tag{5.60}$$

$$\langle \rho_b(x) \rangle = \int_{u_b}^{\infty} \frac{\mathrm{d}\varepsilon}{2\pi v_b^o} \left[f_b(\varepsilon) \left(1 + 2\,\mathrm{Re}\Big\{ e^{2ik_b^o x} S_{bb}(\varepsilon) \Big\} \right) + \sum_{a \in \mathcal{O}(\varepsilon)} f_a(\varepsilon) |\hat{S}_{ba}(\varepsilon)|^2 \right] + \int_{-\infty}^{u_b} \frac{\mathrm{d}\varepsilon}{2\pi}\, e^{-2k_b^c x} \sum_{a \in \mathcal{O}(\varepsilon)} \frac{f_a(\varepsilon)}{v_a^o} |S_{ba}(\varepsilon)|^2 \quad (5.61)$$

Full derivation is in Appendix G. The last term in the above equation cannot be rewritten in terms of the unitary scattering matrix, since the ε-interval makes the b-channel permanently closed, and the whole term would vanish, which is also clear from (5.47). The above equation has a clear new addition compared to the case without induced leads: the last term, which has an exponential decay of particles in closed channels, which is expected.

$$\int_{-\infty}^{u_b} \mathrm{d}\varepsilon\, e^{-2k_b^c x} \sum_{a \in \mathcal{O}(\varepsilon)} \frac{f_a(\varepsilon)}{v_a^o} |S_{ba}(\varepsilon)|^2 = \sum_{a | u_a < u_b} \int_{u_a}^{u_b} \mathrm{d}\varepsilon \frac{f_a(\varepsilon)}{v_a^o} e^{-2k_b^c x} |S_{ba}(\varepsilon)|^2 \quad (5.62)$$

In the end of section 4.1, we found a case for an energy-independent scattering matrix, that required non-induced leads, and we will now calculate the particle density in this case. If all leads are permanently open, the last term above vanish. We found the $N \times N$ scattering matrix to take the form

$$S_{ba} = \frac{2}{N} - \delta_{ba} \quad (5.63)$$

We also assume zero temperature for simplicity.

$$\langle \rho_b^0(x) \rangle = \int_0^{\mu_b} \frac{\mathrm{d}\varepsilon}{v_b^o} \left(1 + 2\,\mathrm{Re}\Big\{ e^{2ik_b^o x} S_{bb} \Big\} \right) + \sum_{a=1}^{N} \int_0^{\mu_a} \mathrm{d}\varepsilon\, \frac{1}{v_a^o} |S_{ba}|^2 \quad (5.64)$$

$$= 2k_{F,b} \left(1 + \frac{2-N}{N} \frac{\sin 2k_{F,b}x}{2k_{F,b}x} \right) + \frac{4}{N^2} \sum_{a=1}^{N} k_{F,a} - \frac{4k_{F,b}}{N} \quad (5.65)$$

with

$$k_{F,a} = \sqrt{2m\mu_a}. \quad (5.66)$$

Also note that at $N = 2$ there is no x dependence, and the particle density would be constant along the two leads, and indeed the scattering matrix in (5.63) has solely zeros on the diagonal, hence no reflection occurs. The particle density right outside the junction, in edge b is

$$\langle \rho_b^0(0) \rangle = \frac{4}{N^2} \sum_{a=1}^{N} k_{F,a} \quad (5.67)$$

The specific oscillation type in equation (5.65) is famously known as Friedel oscillations. The oscillatory part is depicted on figure 9.

$$\langle \rho_b^0(x) \rangle^{\mathrm{osc}} / 2k_{F,b} = 1 + \frac{2-N}{N} \frac{\sin 2k_{F,b}x}{2k_{F,b}x} \quad (5.68)$$

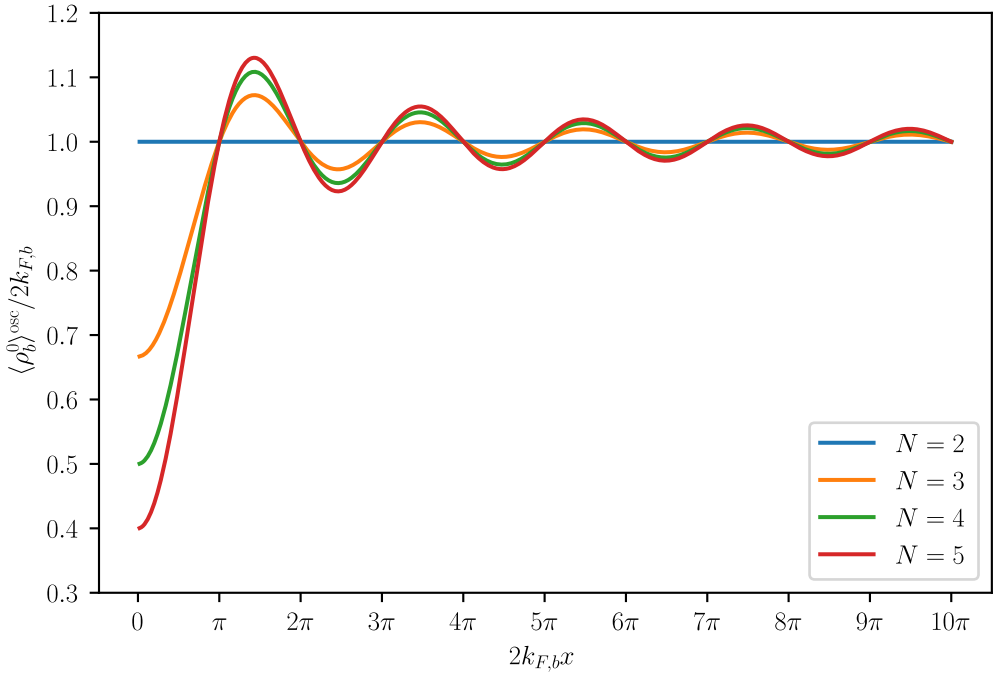


Figure 9: The oscillatory part of the particle density in edge b given by (5.68). The scattering matrix is scale-invariant, and given by (5.63).

Alongside particle density, we can find the heat current κ_b in edge E_b. It is given by [7]

$$\kappa_b(x,t) = \theta_b(x,t) - \mu_b J_b(x,t) \tag{5.69}$$

where

$$\theta_b(x,t) = \frac{1}{4m}\psi_b^\dagger(x,t) R \psi_b(x,t) \tag{5.70}$$

is the energy current, with

$$R = \overleftarrow{\partial}_t\vec{\partial}_x + \overleftarrow{\partial}_x\vec{\partial}_t - \left(\overleftarrow{\partial}_t\overleftarrow{\partial}_x + \vec{\partial}_t\vec{\partial}_x\right) \tag{5.71}$$

and so

$$\theta_b(x,t) = \frac{1}{4m}\iint \frac{\mathrm{d}\varepsilon'\mathrm{d}\varepsilon}{2\pi}\sum_{a',a} c_{a'}^\dagger(\varepsilon')c_a(\varepsilon)\left[\chi_{a'b}^*(x,\varepsilon')e^{i\varepsilon' t}\right] R\left[\chi_{ab}(x,\varepsilon)e^{-i\varepsilon t}\right] \tag{5.72}$$

$$= \frac{i}{4m}\iint \frac{\mathrm{d}\varepsilon'\mathrm{d}\varepsilon}{2\pi}(\varepsilon+\varepsilon')e^{i(\varepsilon'-\varepsilon)t}\sum_{a',a} c_{a'}^\dagger(\varepsilon')c_a(\varepsilon)\chi_{a'b}^*(x,\varepsilon')\mathcal{R}\chi_{ab}(x,\varepsilon) \tag{5.73}$$

and

$$Q_b = \langle \theta_b(x,t) \rangle = \frac{i}{2m} \int_{-\infty}^{\infty} \frac{\mathrm{d}\varepsilon}{2\pi}\, \varepsilon \sum_{a \in \mathcal{O}(\varepsilon)} f_a(\varepsilon) \chi^*_{ab}(x,\varepsilon) \mathcal{R} \chi_{ab}(x,\varepsilon) \tag{5.74}$$

$$= \int_{u_b}^{\infty} \frac{\mathrm{d}\varepsilon}{2\pi}\, \varepsilon \sum_{a \in \mathcal{O}(\varepsilon)} [\delta_{ab} - |\hat{S}_{ab}(\varepsilon)|^2] f_a(\varepsilon) \tag{5.75}$$

$$= \int_{u_b}^{\infty} \frac{\mathrm{d}\varepsilon}{2\pi}\, \varepsilon \sum_{a \in \mathcal{O}(\varepsilon)} [f_b(\varepsilon) - f_a(\varepsilon)]\, |\hat{S}_{ba}(\varepsilon)|^2 \tag{5.76}$$

which is very similar in structure to I_b^{part} in (5.46c), and neither is position or time dependent. We can then find the heat current

$$\kappa_b = \frac{i}{2m} \iint \frac{\mathrm{d}\varepsilon\, \mathrm{d}\varepsilon'}{2\pi} \left(\frac{\varepsilon + \varepsilon'}{2} - \mu_b \right) e^{i(\varepsilon' - \varepsilon)t} \sum_{a',a} c^\dagger_{a'}(\varepsilon') c_a(\varepsilon) \chi^*_{a'b}(x,\varepsilon') \mathcal{R} \chi_{ab}(x,\varepsilon) \tag{5.77}$$

and then

$$I_b^{\text{heat}} = \langle \kappa_b \rangle = Q_b - \mu_b I_b^{\text{part}} \tag{5.78}$$

$$= \int_{u_b}^{\infty} \frac{\mathrm{d}\varepsilon}{2\pi} (\varepsilon - \mu_b) \sum_{a \in \mathcal{O}(\varepsilon)} [f_b(\varepsilon) - f_a(\varepsilon)]\, |\hat{S}_{ba}(\varepsilon)|^2. \tag{5.79}$$

5.3.1 Conservation laws and symmetry

At this stage, we can check various conservation laws, like the continuity equation for particles and Kirchhoff's law at operator form.

$$\sum_{b=1}^{N} J_b(0) = 0 \tag{5.80}$$

and since both $\psi_b(x)$ and $\psi_b^\dagger(x)$ are fields on the graph G, they have to satisfy the boundary conditions laid out in section 3 in (3.35):

$$J_b(0) = \lim_{x \to 0^+} \frac{i}{2m} \left(\psi_b^\dagger(x) \partial_x \psi_b(x) - \partial_x \psi_b^\dagger(x)\, \psi_b(x) \right) \tag{5.81a}$$

$$\sum_{b=1}^{N} J_b(0) = \frac{i}{2m} \sum_{b=1}^{N} \left(\psi_b^\dagger(0) \partial_x \psi_b(0) - \partial_x \psi_b^\dagger(0)\, \psi_b(0) \right) \tag{5.81b}$$

$$= 0. \tag{5.81c}$$

Kirchhoff's law for conductance

$$\sum_{b=1}^{N} G_{bb'}(\mu_{b'}) = e^2 \int_{u_{b'}}^{\infty} \mathrm{d}\varepsilon \sum_{b \in \mathcal{O}(\varepsilon)} \left[\delta_{bb'} - |\hat{S}_{bb'}(\varepsilon)|^2 \right] \frac{\partial f_{b'}(\varepsilon)}{\partial \mu_{b'}} = 0, \tag{5.82}$$

holds as well for all b'.

The continuity equation:

$$0 = \partial_t \rho_b(x,t) - \partial_x J_b(x,t) = \iint \frac{\mathrm{d}\varepsilon\ \mathrm{d}\varepsilon'}{(2\pi)^2} \sum_{\substack{a\in\mathcal{O}(\varepsilon)\\ a'\in\mathcal{O}(\varepsilon')}} c^\dagger_{a'}(\varepsilon') c_a(\varepsilon)$$
$$\times \left\{ \chi^*_{a'b}(x,\varepsilon')\chi_{ab}(x,\varepsilon)\partial_t e^{i(\varepsilon'-\varepsilon)t} - \frac{i}{2m}\left[\chi^*_{a'b}(x,\varepsilon')\partial_x^2\chi_{ab}(x,\varepsilon) - \partial_x^2\chi^*_{a'b}(x,\varepsilon')\ \chi_{ab}(x,\varepsilon)\right] e^{i(\varepsilon'-\varepsilon)t} \right\} \tag{5.83}$$

with the brackets equals

$$\{\cdots\} = ie^{i(\varepsilon'-\varepsilon)t}\chi^*_{a'b}(x,\varepsilon')\chi_{ab}(x,\varepsilon)\left((\varepsilon'-\varepsilon) - \left[-\frac{k_b^2}{2m} + \frac{(k_b')^2}{2m}\right]\right) = 0 \tag{5.84}$$

since $\varepsilon - k_b^2/2m = \varepsilon' - (k_b')^2/2m = u_b$. It also holds trivially for expectation values since $\langle\rho_b(x,t)\rangle$ is time-independent, and the current $\langle J_b(x,t)\rangle = I_b$ is position independent.

6 Quantum quench protocols

We will now explore what happens as we quench from the non-induced wire system, to a system with induced wires and vice versa. Doing so, we will consider two protocols, as quickly mentioned in the introduction. The two systems with and without induced wires are summarised below:

- System one $\mathcal{S}_1$: The non-equilibrium system with a non-zero temperature and potential at the reservoirs. A constant current is present, and the unitary scattering matrix $S(k)$ is given by (2.26). This system is nicely explored in [6].

- The non-equilibrium system with a non-zero temperature and potential at the reservoirs as well as induced potentials in the leads. A constant current is present, and the unitary scattering matrix $\hat{S}(\varepsilon)$ is given by (3.45), and here the energy is a good quantum number.

Pure system two never occurs in reality, as one always turn on the voltage/system at some finite point in time, and the calculation of the observables have assumed that the system has been the same for all times. A way to simulate system two is thus by a quench. We will discuss two quench protocols, which in both cases, at time $t = 0$ a parameter in the Hamiltonian changes, and the ground state before the quench, is thus not a ground state anymore and will now evolve according to a new Hamiltonian. This evolution is usually highly non-trivial. One can then asks if the system, after a sufficiently long time, thermalizes into a steady state? Inspired by [14], we make the following definitions of quench protocols, we will explore:

1. ***μ* quenches**:
   For $t < 0$ the edges are connected to the scatterer, there is a global chemical potential μ at the reservoirs and the induced potentials in the leads are all zero, thus the particle density across

each lead is equal. The current vanish, and the unitary scattering matrix $S(k)$ can in general be non-trivial, and is given by (2.26). When $t \geq 0$, the induced potentials turn on, the reservoirs are disconnected and the unitary scattering matrix $\hat{S}(\varepsilon)$ now depend on the induced potentials, and the current is non-zero.

2. **Density quenches**:
   For $t < 0$ the scatterer and the leads are disconnected, such that there is no exchange of particles between leads, but the leads are connected to the reservoirs, so the induced potentials in the leads are different. As $t \geq 0$, one connects the scatterer and the leads, and disconnect the reservoirs, and the system evolves according to $H_<$.

Thus in the end, one might expect that NESSs are reached in the μ and density quench with a scattering matrix given by $\hat{S}(\varepsilon)$ (3.45) and $S(k)$, (2.26) respectively.

The temporal evolution of the quench is as follows: At time zero we turn on the induced leads, and disconnect the reservoirs. As this is done instantaneously, the signal has to propagate along the edges at the speed of "sound" and opens a light-cone, to update the remaining wire with the information that the leads now indeed has a potential. If the system is finite, the electric current, that is within this light-cone, is thus in a quasi steady state, since the signal will re-bounce on the edge of the wire and propagate back and disrupt the steady state. It is in this non-equilibrium quasi stead state (NEQSS) we wish to calculate transport properties. Of course, since reservoirs are no longer present, after a sufficiently long times the system will settle to an actual steady state whose current is zero.

The evidence for that the density quench protocol finds a NEQSS given by a Landauer Büttiker form is convincingly given in [14], [15]. Both phenomenological and numerical arguments have been made, as well as tight binding examples verifying it. We will thus only focus on the μ quench in the following.

6.1 The μ quench

For the μ quench, we start in $t < 0$ with no induced potentials and thus all channels are open, and at $t \geq 0$, they are present and the possibility of a closed channel is present. So the two Hamiltonians we will need are

$$H_< = \sum_{j=1}^{N} \frac{-\partial_{j,x}^2}{2m} \tag{6.1}$$

$$H_> = \sum_{j=1}^{N} \frac{-\partial_{j,x}^2}{2m} + u_j \tag{6.2}$$

where the subscripts $<$ and $>$ indicate in which time-regime Hamiltonians are acting in: $H_>$ is present for $t \geq 0$ and $H_<$ for $t < 0$. However, the Hamiltonians in second quantisation are the one we will

work with and are

$$H_< = \int_0^\infty \mathrm{d}k \sum_{a=1}^{N} \tilde{c}_a^\dagger(k)\tilde{c}_a(k)\frac{k^2}{2m} \tag{6.3a}$$

$$H_> = \int_{-\infty}^\infty \mathrm{d}\varepsilon \sum_{a\in\mathcal{O}(\varepsilon)} c_a^\dagger(\varepsilon)c_a(\varepsilon)\varepsilon \tag{6.3b}$$

From now on, we will denote with a tilde $\tilde{}$ quantities in the $t<0$ regime. As we connect the reservoirs, we allow for a channel to get closed: so the two wavefunctions in the two regimes are, respectively,

$$\tilde{\chi}_{ab}(x,k) = \left(e^{-ikx}\delta_{ab} + e^{ikx}\tilde{S}_{ba}(k)\right), \quad a=1,...,N \tag{6.4a}$$

$$\chi_{a'b}(x,\varepsilon') = \frac{1}{\sqrt{v_{a'}^{o\prime}}}\left(e^{-ik_{a'}^{o\prime}x}\delta_{a'b} + e^{i(k_b^{o\prime}+ik_b^{c\prime})x}S_{ba'}(\varepsilon')\right), \quad a'=1,...,n(\varepsilon') \tag{6.4b}$$

where we have inserted normalisation explicitly. In the matrix $\tilde{S}$ the momentum is still a scalar, and in S momentum is a matrix. We naturally define the overlap of the wavefunctions in the two regimes as the following big mess

$$\Gamma_{ab}(k,\varepsilon) = \langle\tilde{\chi}_a(k)|\chi_b(\varepsilon)\rangle = \sum_{j=1}^{N}\int_0^\infty \mathrm{d}x\ \tilde{\chi}_{aj}^*(x,k)\chi_{bj}(x,\varepsilon) \tag{6.5}$$

$$\begin{aligned}=&\frac{1}{\sqrt{v_b^o}}\Bigg[\pi\delta(k-k_b^o)\delta_{ab} + \delta_{ab}\frac{i}{k-k_b^o} + \pi\sum_{j\in\mathcal{O}(\varepsilon)}\delta(k-k_j^o)\tilde{S}_{ja}^*(k)S_{jb}(\varepsilon) + \\ &\frac{i}{k+k_b}S_{ab}(\varepsilon) - \tilde{S}_{ab}^\dagger(k)\frac{i}{k+k_b^o} + \sum_{j=1}^{N}\tilde{S}_{aj}^\dagger(k)\frac{i}{k_j-k}S_{jb}(\varepsilon)\Bigg]\end{aligned} \tag{6.6}$$

again with

$$k_b = k_b^o + ik_b^c = \sqrt{2m(\varepsilon-u_b)} \tag{6.7}$$

being the entries of the $N\times N$ diagonal matrix $\boldsymbol{k}'$, not to be confused by $k=\sqrt{2m\varepsilon}$, that is the momentum for the non-induced case. Since $a=1,...,N$ and $a'=1,...,n(\varepsilon')$ then $k'_{a'}=k_{a'}^{o\prime}$. The transformation from creation and annihilation operators from $t<0$ and $t>0$ is then

$$\tilde{c}_a^\dagger(k) = \frac{1}{\sqrt{L}}\int \mathrm{d}\varepsilon \sum_{b\in\mathcal{O}(\varepsilon)}\Gamma_{ab}^*(k,\varepsilon)c_b^\dagger(\varepsilon) \tag{6.8a}$$

$$\tilde{c}_a(k) = \frac{1}{\sqrt{L}}\int \mathrm{d}\varepsilon \sum_{b\in\mathcal{O}(\varepsilon)}\Gamma_{ab}(k,\varepsilon)c_b(\varepsilon) \tag{6.8b}$$

and the inverted version is

$$c_a^\dagger(\varepsilon) = \sqrt{L}\int \mathrm{d}k \sum_{b=1}^{N}\Gamma_{ba}(k,\varepsilon)\tilde{c}_b^\dagger(k) \tag{6.9a}$$

$$c_a(\varepsilon) = \sqrt{L}\int \mathrm{d}k \sum_{b=1}^{N}\Gamma_{ba}^*(k,\varepsilon)\tilde{c}_b(k) \tag{6.9b}$$

with $\Gamma^*_{a'a}(\varepsilon',\varepsilon) = (\Gamma_{a'a}(\varepsilon',\varepsilon))^*$. Here $c(\varepsilon)$ has $1/\sqrt{\mathrm{E}}$ and $\tilde{c}(k)$ is unit-less and Γ has $\sqrt{\mathrm{L/E}}$. This makes

$$\langle \tilde{c}^\dagger_{a'}(k')\tilde{c}_a(k)\rangle = \frac{2\pi}{L}\delta_{a'a}\delta(k'-k). \tag{6.10}$$

Imagining the evolution of the μ quench, it is natural to propose that as $t\to\infty$ the system settles to the known L.B.-system with a NESS given by (5.46c). This is now what we would like to explore. Explicitly we propose that

$$W_b(x) = \lim_{T\to\infty}\frac{1}{T}\int_0^T \mathrm{d}t\, \langle\psi_{GS}|\, e^{iH_{>}t}J_b(x)e^{-iH_{>}t}\,|\psi_{GS}\rangle = \text{L.B.-like}, \tag{6.11}$$

The ground-state above is given by

$$|\psi_{GS}\rangle = \bigotimes_{0\le\varepsilon(k)\le\mu}\prod_{a=1}^N \tilde{c}^\dagger_a(k)\,|0\rangle \tag{6.12}$$

where $|0\rangle$ is the vacuum state, i.e. no particles. Since the ground-state is completely filled up to energy μ, we cannot create particles with energy $\le\mu$ since there's no room nor remove ones with energy $>\mu$ since there are none. The Fermi energy is $k_F = \sqrt{2m\mu}$

$$\tilde{c}_a(k>k_F)\,|\psi_{GS}\rangle = 0 \tag{6.13a}$$

$$\tilde{c}^\dagger_a(k\le k_F)\,|\psi_{GS}\rangle = 0 \tag{6.13b}$$

The time evolution of the electric current was found earlier in (5.45):

$$J_b(x,t) = e^{iH_{>}t}J_b(x)e^{-iH_{>}t} = \frac{i}{2m}\iint\frac{\mathrm{d}\varepsilon'\mathrm{d}\varepsilon}{2\pi}e^{i(\varepsilon'-\varepsilon)t}\sum_{a',a}c^\dagger_{a'}(\varepsilon')c_a(\varepsilon)\,\chi^*_{a'b}(x,\varepsilon')\mathcal{R}\chi_{ab}(x,\varepsilon). \tag{6.14}$$

So

$$W_b(x) = \lim_{T\to\infty}\frac{1}{T}\int_0^T\mathrm{d}t\iint\frac{\mathrm{d}\varepsilon'\mathrm{d}\varepsilon}{2\pi}\frac{ie^{i(\varepsilon'-\varepsilon)t}}{2m}\sum_{a',a}\chi^*_{a'b}(x,\varepsilon')\mathcal{R}\chi_{ab}(x,\varepsilon)\,\langle\psi_{GS}|\,c^\dagger_{a'}(\varepsilon')c_a(\varepsilon)\,|\psi_{GS}\rangle \tag{6.15}$$

where

$$\langle\psi_{GS}|\,c^\dagger_{a'}(\varepsilon')c_a(\varepsilon)\,|\psi_{GS}\rangle = L\sum_{b',b=1}^N\iint_0^{k_F}\mathrm{d}k\,\mathrm{d}k'\,\Gamma_{b'a'}(k',\varepsilon')\Gamma^*_{ba}(k,\varepsilon)\,\langle\psi_{GS}|\,\tilde{c}^\dagger_{b'}(k')\tilde{c}_b(k)\,|\psi_{GS}\rangle \tag{6.16}$$

$$= 2\pi\sum_{b=1}^N\int_0^{k_F}\mathrm{d}k\,\Gamma_{ba'}(k,\varepsilon')\Gamma^*_{ba}(k,\varepsilon)f_b(\varepsilon(k)-\mu_b) \tag{6.17}$$

and we define

$$X_{a'a}(\varepsilon',\varepsilon) = \sum_{b=1}^N\int_0^{k_F}\mathrm{d}k\,\Gamma_{ba'}(k,\varepsilon')\Gamma^*_{ba}(k,\varepsilon)f_b(\varepsilon(k)-\mu_b). \tag{6.18}$$

So

$$W_b(x) = \frac{i}{2m}\lim_{T\to\infty}\frac{1}{T}\int_0^T\mathrm{d}t\iint\mathrm{d}\varepsilon'\mathrm{d}\varepsilon\,e^{i(\varepsilon'-\varepsilon)t}\sum_{a',a}\chi^*_{a'b}(x,\varepsilon')\mathcal{R}\chi_{ab}(x,\varepsilon)X_{a'a}(\varepsilon',\varepsilon) \tag{6.19}$$

After the quench one can then, for simplicity, assume one turns on a single potential u in channel ℓ. This one channel then acts as a reservoir, and we postulate that the conductance is given in terms of this shift in energy $\mu+u$.

$$G^{\text{quench}}_{b\ell} = G_{b\ell}(\mu_\ell = u+\mu),\quad \forall b. \tag{6.20}$$

7 Conclusion and outlook

A quantum star graph is a network of nano-wires with an arbitrary number of leads and channels, connected to a single vertex. Each wire is connected to a thermal reservoir, and the system is away from equilibrium if, in general, a current flows. At the vertex of the graph is a scatterer that is assumed to be point-like and non-interacting, that, in a physical system, can take the role as an impurity, a quantum device or the alike. This scatterer is mathematically described by a unitary scattering matrix $S(k)$, that depends on the momentum k of the incoming electron wave. Furthermore, the exact form of S, is found in terms of the boundary conditions that each wavefunction, in the leads, make at the vertex. Such a system has been studied to great detail by e.g. M. Mintchev in [5]–[7].

We now consider the leads to be induced with a constant potential. This effect is realised as an intrinsic process by the reservoir-lead coupling, or from an external source. Because of the electron's presence, a potential in the leads is created. Calculating the electron's contribution to the potential is done self-consistently, by solving Schrödinger-Poisson's equations. An external source to induce a potential can take the form of an electrostatic potential, that may come from a wire that is in proximity to the wire of the graph. The potentials in the wire acts as impenetrable walls for electrons with inadequate energy, hence leads to the concept of open and closed channels. Because of this novelty, wavefunctions in the leads and the unitary scattering matrix changes accordingly. We prove the orthogonality of the wavefunctions, and the unitarity of the new scattering matrix.

Equipped with the new scattering matrix formalism for induced potentials, we create a quantum field theory on the graph G, upon which, observables like electric current, particle density, differential conductance and heat current is calculated. We find that the electric current is both time and position independent, alluding to the fact that this indeed is a non-equilibrium steady state. For a scale invariant scattering matrix, we find that the particle density make Friedel oscillations along each lead. Such oscillation patterns are typical in metallic or semi-conductor systems with a point-like impurity.

Considering the two regimes with and without induced potentials, we briefly explored a quantum quench protocol in which a system starts without potentials, and then suddenly the potentials are turned on. The signal of this sudden change of Hamiltonian propagates throughout the graph, and before the signal hits the edges of the graph, we postulate that there exists a non-equilibrium quasi steady state, and that the long-time limit of the current will approach the Landauer-Büttiker value.

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Appendices

A Existence of the scattering matrix for real momentum-matrix

We will now show that $A^\dagger - i\boldsymbol{k}B^\dagger$ for $\boldsymbol{k}$ a real (and non-zero), diagonal, matrix, indeed is invertible inspired by [10].

$$\det\left(A^\dagger - i\boldsymbol{k}B^\dagger\right) = \det\left(\sqrt{\boldsymbol{k}}\right)\det\left(\sqrt{\boldsymbol{k}}^{-1}A^\dagger - i\sqrt{\boldsymbol{k}}B^\dagger\right) = 0. \tag{A.1}$$

Showing that $\sqrt{\boldsymbol{k}}^{-1}A^\dagger - i\sqrt{\boldsymbol{k}}B^\dagger$ is invertible is equivalent to showing $A^\dagger - i\boldsymbol{k}B^\dagger$ is invertible, since $\det\sqrt{\boldsymbol{k}} \neq 0$. There exists a non-zero vector v such that

$$\left(\sqrt{\boldsymbol{k}}^{-1}A^\dagger - i\sqrt{\boldsymbol{k}}B^\dagger\right)v = 0 \tag{A.2}$$

$$0 = \left\langle v, \left(A\sqrt{\boldsymbol{k}}^{-1} + iB\sqrt{\boldsymbol{k}}\right)\left(\sqrt{\boldsymbol{k}}^{-1}A^\dagger - i\sqrt{\boldsymbol{k}}B^\dagger\right)v\right\rangle \tag{A.3}$$

$$= \left\langle \sqrt{\boldsymbol{k}}^{-1}A^\dagger v, \sqrt{\boldsymbol{k}}^{-1}A^\dagger v\right\rangle + \left\langle \sqrt{\boldsymbol{k}}B^\dagger v, \sqrt{\boldsymbol{k}}B^\dagger v\right\rangle \tag{A.4}$$

concluding that

$$\sqrt{\boldsymbol{k}}^{-1}A^\dagger v = \sqrt{\boldsymbol{k}}B^\dagger v = 0, \tag{A.5}$$

$$A^\dagger v = B^\dagger v = 0. \tag{A.6}$$

Now notice that, since the composite matrix (A, B) has maximal rank, namely N, there is at least one solution to

$$A\phi + B\phi' = \psi \tag{A.7}$$

for (ϕ, ϕ'), where $\psi \in \mathbb{C}^N$. Now

$$0 = \langle\phi, A^\dagger v\rangle + \langle\phi', B^\dagger v\rangle = \langle A\phi + B\phi', v\rangle \tag{A.8}$$

The only solution is to have $v = 0$, which is contradictory to the initial assumption. Thus $A^\dagger - i\boldsymbol{B}^\dagger$ and $\sqrt{\boldsymbol{k}}^{-1}A^\dagger - i\sqrt{\boldsymbol{k}}B^\dagger$ is invertible. The invertibility of the hermitian conjugated version is proven similarly.

B Wavefunctions are orthogonal for a real momentum-matrix

We define the state vector $|\chi_a(\varepsilon)\rangle$ with the label a to indicate in which lead we're inserting a wave, with energy ε. We wish to show that

$$\langle\chi_{a'}(\varepsilon')|\chi_a(\varepsilon)\rangle = \sum_{b=1}^{N}\int_0^\infty \mathrm{d}x\ \chi^*_{a'b}(x,\varepsilon')\chi_{ab}(x,\varepsilon) = 2\pi\delta_{a'a}\delta(\varepsilon' - \varepsilon) \tag{B.1}$$

with

$$\chi_{ab}(x,\varepsilon) = \langle b, x|\chi_a(\varepsilon)\rangle \tag{B.2}$$

where we have inserted that

$$1 = \sum_{b=1}^{N} \int_0^\infty \mathrm{d}x \, |b, x\rangle \, \langle b, x| \tag{B.3}$$

$$\langle \chi_{a'}(\varepsilon')|\chi_a(\varepsilon)\rangle = \sum_j \int \mathrm{d}x \, (e^{ik'_{a'}x}\delta_{ja'} + e^{-ik'_j x} S^*_{ja'}(\varepsilon'))(e^{-ik_a x}\delta_{ja} + e^{ik_j x} S_{ja}(\varepsilon)) \tag{B.4}$$

Expanding, we get four contributions, and using that

$$\int_0^\infty \mathrm{d}x \, e^{ikx} = \pi\delta(k) + \frac{i}{k}, \quad k \in \mathbb{R} \tag{B.5}$$

we get that those are

$$F^1_{aa'} = \sum_j \int \mathrm{d}x \, e^{i(k'_{a'} - k_a)x} \delta_{ja}\delta_{ja'} = \delta_{aa'} \left(\pi\delta(k'_a - k_a) + \frac{i}{k'_a - k_a} \right) \tag{B.6a}$$

$$F^2_{aa'} = \sum_j \int \mathrm{d}x \, e^{i(k'_{a'} + k_j)x} \delta_{ja'} S_{ja}(\varepsilon) = S_{a'a}(\varepsilon) \left(\pi\delta(k'_{a'} + k_{a'}) + \frac{i}{k'_{a'} + k_{a'}} \right) \tag{B.6b}$$

$$F^3_{aa'} = \sum_j \int \mathrm{d}x \, e^{-i(k'_j + k_a)x} S^*_{ja'}(\varepsilon')\delta_{ja} = S^*_{aa'}(\varepsilon') \left(\pi\delta(k'_a + k_a) - \frac{i}{k'_a + k_a} \right) \tag{B.6c}$$

$$F^4_{aa'} = \sum_j \int \mathrm{d}x \, e^{i(k_j - k'_j)x} S^*_{ja'}(\varepsilon') S_{ja}(\varepsilon) = \sum_j S^\dagger_{a'j}(\varepsilon') S_{ja}(\varepsilon) \left(\pi\delta(k'_j - k_j) - \frac{i}{k'_j - k_j} \right) \tag{B.6d}$$

Since all $k_i, k'_i > 0$

$$\delta(k'_{a'} + k_{a'}) = \delta(k'_a + k_a) = 0. \tag{B.7}$$

Now, for $\delta(k'_j - k_j)$, we need $\partial(k'_j - k_j)/\partial\varepsilon|_{\varepsilon_0}$, with $\varepsilon_0 = \varepsilon'$. We introduce velocities

$$v_a^{-1} = \frac{\partial k_a(\varepsilon)}{\partial\varepsilon}|_{\varepsilon=\varepsilon'} = \frac{m}{\sqrt{2m(\varepsilon' - \mu_a)}} = m/k_a. \tag{B.8}$$

So

$$\delta(k_a - k'_a) = \delta(\varepsilon - \varepsilon')v_a. \tag{B.9}$$

By setting

$$v = \mathrm{diag}(v_1, ..., v_N), \quad u = \mathrm{diag}\left(\frac{1}{k'_1 - k_1}, ..., \frac{1}{k'_N - k_N} \right), \quad \bar{u} = \mathrm{diag}\left(\frac{1}{k'_1 + k_1}, ..., \frac{1}{k'_N + k_N} \right), \tag{B.10}$$

then the F's can be written in matrix form as

$$F^1 = \pi v\delta(\varepsilon - \varepsilon') + iu \tag{B.11}$$

$$F^2 = i\bar{u}S(\varepsilon) \tag{B.12}$$

$$F^3 = -iS^\dagger(\varepsilon')\bar{u} \tag{B.13}$$

$$F^4 = \pi\delta(\varepsilon - \varepsilon')S^\dagger(\varepsilon')vS(\varepsilon) - iS^\dagger(\varepsilon')uS(\varepsilon). \tag{B.14}$$

So with $F_{a'a} = \langle \chi_{a'}(\varepsilon')|\chi_a(\varepsilon)\rangle$

$$F = \pi\delta(\varepsilon - \varepsilon')v + iu + i\bar{u}S(\varepsilon) - iS^\dagger(\varepsilon')\bar{u} + \pi\delta(\varepsilon - \varepsilon')S^\dagger(\varepsilon')vS(\varepsilon) - iS^\dagger(\varepsilon')uS(\varepsilon). \tag{B.15}$$

We now calculate the sum of terms proportional to $\delta(\varepsilon-\varepsilon')$:

$$\pi\delta(\varepsilon-\varepsilon')v'+\pi\delta(\varepsilon-\varepsilon')S^\dagger(\varepsilon')vS(\varepsilon)=\pi\delta(\varepsilon-\varepsilon')v'\Big[\mathbf{1}_N+{v'}^{-1}S^\dagger(\varepsilon')vS(\varepsilon)\Big]\overset{!}{\propto}\mathbf{1}_N\delta(\varepsilon'-\varepsilon). \quad \text{(B.16)}$$

For the wavefunctions to be orthogonal, we want ${v'}^{-1}S^\dagger(\varepsilon')vS(\varepsilon)=\mathbf{1}$, meaning (since v is proportional to k, and $\varepsilon'=\varepsilon$)

$$\sqrt{k}^{-1}S^\dagger(\varepsilon)\sqrt{k}\sqrt{k}S(\varepsilon)\sqrt{k}^{-1}=\mathbf{1}_N \quad \text{(B.17)}$$

we then define the unitary matrix $\hat{S}$ as

$$\hat{S}(\varepsilon)=\sqrt{k}S(\varepsilon)\sqrt{k}^{-1}=-\left(A\sqrt{k}^{-1}+iB\sqrt{k}\right)^{-1}\left(A\sqrt{k}^{-1}-iB\sqrt{k}\right). \quad \text{(B.18)}$$

Equation (B.17) simplifies to the unitarity condition

$$\hat{S}^\dagger(\varepsilon)\hat{S}(\varepsilon)=\mathbf{1}_N. \quad \text{(B.19)}$$

We now prove that $\hat{S}$ is unitary, by using the explicit form of S from (2.26), and using that $AB^\dagger=BA^\dagger$

$$\hat{S}=-\left(A\sqrt{k}^{-1}+iB\sqrt{k}\right)^{-1}\left(A\sqrt{k}^{-1}-iB\sqrt{k}\right) \quad \text{(B.20)}$$

$$=-\left(\sqrt{k}^{-1}A^\dagger-i\sqrt{k}B^\dagger\right)\left(\sqrt{k}^{-1}A^\dagger-i\sqrt{k}B^\dagger\right)^{-1}\left(A\sqrt{k}^{-1}+iB\sqrt{k}\right)^{-1}\left(A\sqrt{k}^{-1}-iB\sqrt{k}\right) \quad \text{(B.21)}$$

$$=-\left(\sqrt{k}^{-1}A^\dagger-i\sqrt{k}B^\dagger\right)\left[Ak^{-1}A^\dagger+BkB^\dagger\right]^{-1}\left(A\sqrt{k}^{-1}-iB\sqrt{k}\right) \quad \text{(B.22)}$$

$$\hat{S}^\dagger=-\left(\sqrt{k}^{-1}A^\dagger+i\sqrt{k}B^\dagger\right)\left[Ak^{-1}A^\dagger+BkB^\dagger\right]^{-1}\left(A\sqrt{k}^{-1}+iB\sqrt{k}\right) \quad \text{(B.23)}$$

$$\hat{S}^{-1}=-\left(A\sqrt{k}^{-1}-iB\sqrt{k}\right)^{-1}\left(A\sqrt{k}^{-1}+iB\sqrt{k}\right) \quad \text{(B.24)}$$

$$=-\left(\sqrt{k}^{-1}A^\dagger+i\sqrt{k}B^\dagger\right)\left(\sqrt{k}^{-1}A^\dagger+i\sqrt{k}B^\dagger\right)^{-1}\left(A\sqrt{k}^{-1}-iB\sqrt{k}\right)^{-1}\left(A\sqrt{k}^{-1}+iB\sqrt{k}\right) \quad \text{(B.25)}$$

$$=-\left(\sqrt{k}^{-1}A^\dagger+i\sqrt{k}B^\dagger\right)\left[Ak^{-1}A^\dagger+BkB^\dagger\right]^{-1}\left(A\sqrt{k}^{-1}+iB\sqrt{k}\right) \quad \text{(B.26)}$$

showing that $\hat{S}^{-1}=\hat{S}^\dagger$, so $\hat{S}$ is a unitary matrix. We also note

$$\hat{S}_{A,B}(\varepsilon)=\hat{S}^\top_{A^*,B^*}(\varepsilon) \quad \text{(B.27)}$$

which can be seen directly from above. The notation $\hat{S}_{A^*,B^*}(\varepsilon)$ simply means $\hat{S}(\varepsilon)=\hat{S}_{A,B}(\varepsilon)$ with $A\to A^*$ and $B\to B^*$ and the star * meaning complex conjugation.

The remaining terms that has to cancel for orthogonality are

$$f=u+\bar{u}S(k)-S^\dagger(k')\bar{u}-S^\dagger(k')uS(k) \quad \text{(B.28)}$$

$$=u+\bar{u}\sqrt{k}^{-1}\hat{S}(k)\sqrt{k}-\sqrt{k'}\hat{S}^\dagger(k')\sqrt{k'}^{-1}\bar{u}-\sqrt{k'}\hat{S}^\dagger(k')\sqrt{k'}^{-1}u\sqrt{k}^{-1}\hat{S}(k)\sqrt{k} \quad \text{(B.29)}$$

$$=u+\bar{u}\sqrt{k}^{-1}\hat{S}(k)\sqrt{k}-\sqrt{k'}\hat{S}(-k')\sqrt{k'}^{-1}\bar{u}-\sqrt{k'}\hat{S}(-k')\sqrt{k'}^{-1}u\sqrt{k}^{-1}\hat{S}(k)\sqrt{k} \quad \text{(B.30)}$$

We will now prove that $f = 0$, by introducing $\hat{T}$ inspired by [5].

$$\hat{S}(\varepsilon) = \mathbf{1} + i\hat{T}(\varepsilon) \tag{B.31}$$

$$\hat{S}^\dagger(\varepsilon) = \mathbf{1} - i\hat{T}^\dagger(\varepsilon) \tag{B.32}$$

This makes

$$i\hat{T}(\varepsilon) = \hat{S}(\varepsilon) - \mathbf{1} \tag{B.33}$$

$$= -\left(A\sqrt{k}^{-1} + iB\sqrt{k}\right)^{-1}\left((A\sqrt{k}^{-1} - iB\sqrt{k}) + (A\sqrt{k}^{-1} + iB\sqrt{k})\right) \tag{B.34}$$

$$= -2\left(A\sqrt{k}^{-1} + iB\sqrt{k}\right)^{-1} A\sqrt{k}^{-1} \tag{B.35}$$

$$\hat{T}(\varepsilon) = 2i\left(A\sqrt{k}^{-1} + iB\sqrt{k}\right)^{-1} A\sqrt{k}^{-1} \tag{B.36}$$

$$\hat{T}^\dagger(\varepsilon') = -2i\sqrt{k'}^{-1} A^\dagger\left(\sqrt{k'}^{-1} A^\dagger - i\sqrt{k'}B^\dagger\right)^{-1}. \tag{B.37}$$

We now apply (B.27) with

$$\left(\mathbf{1} + i\hat{T}(\varepsilon)\right)^\top = \mathbf{1} + i\hat{T}^\top(\varepsilon) \tag{B.38}$$

$$\hat{T}_{A,B}(\varepsilon) = \hat{T}^\top_{A^*,B^*}(\varepsilon) \tag{B.39}$$

go get the two version of $\hat{T}$

$$\hat{T}(\varepsilon) = 2i\left(A\sqrt{k}^{-1} + iB\sqrt{k}\right)^{-1} A\sqrt{k}^{-1} \tag{B.40}$$

$$= 2i\sqrt{k}^{-1} A^\dagger\left(\sqrt{k}^{-1} A^\dagger + i\sqrt{k}B^\dagger\right)^{-1} \tag{B.41}$$

$$\hat{T}^\dagger(\varepsilon') = -2i\sqrt{k'}^{-1} A^\dagger\left(\sqrt{k'}^{-1} A^\dagger - i\sqrt{k'}B^\dagger\right)^{-1} \tag{B.42}$$

$$= -2i\left(A\sqrt{k'}^{-1} - iB\sqrt{k'}\right)^{-1} A\sqrt{k'}^{-1} \tag{B.43}$$

Thus

$$if = -\sqrt{k'}\hat{T}'\bar{u}\sqrt{k'}^{-1} - \sqrt{k}^{-1}\bar{u}\hat{T}\sqrt{k} + \sqrt{k}u\hat{T}\sqrt{k}^{-1} - \sqrt{k'}\hat{T}'u\sqrt{k'}^{-1} - i\sqrt{k'}\hat{T}'\sqrt{k'}^{-1}u\sqrt{k}^{-1}\hat{T}\sqrt{k} \tag{B.44}$$

$$= -T'\bar{u} - \bar{u}T + uT - T'u - iT'uT \tag{B.45}$$

with $\hat{T}$ denoting $\hat{T}(\varepsilon)$ and $\hat{T}'$, $\hat{T}^\dagger(\varepsilon')$ and similarly for T which follows the same transformation as S:

$$\hat{T}(\varepsilon) = \sqrt{k}T(\varepsilon)\sqrt{k}^{-1} \tag{B.46}$$

such that

$$T(\varepsilon) = 2i\left(A + iBk\right)^{-1} A = 2ik^{-1}A^\dagger\left(A^\dagger + ikB^\dagger\right)^{-1} k \tag{B.47}$$

$$T^\dagger(\varepsilon') = -2iA^\dagger\left(A^\dagger - ik'B^\dagger\right)^{-1} = -2ik'\left(A - iBk'\right)^{-1} Ak'^{-1}. \tag{B.48}$$

Introduce

$$\kappa^{-1} = k'^2 - k^2 = 2m(\varepsilon' - \mu) - 2m(\varepsilon - \mu) = 2m\Delta\varepsilon \tag{B.49}$$

which is proportional to the identity. $\Delta\varepsilon = \varepsilon' - \varepsilon$. Now

$$\begin{aligned}
if &= -T'(\bar{u} + u) + (u - \bar{u})T - iT'uT && \text{(B.50)}\\
&= 2ik' \left(A - iBk'\right)^{-1} Ak'^{-1}(\bar{u} + u)k^{-1} \left(A^\dagger + ikB^\dagger\right) \left(A^\dagger + ikB^\dagger\right)^{-1} k && \text{(B.51)}\\
&+ 2ik' \left(A - ik'B\right)^{-1} \left(A - ik'B\right) k'^{-1}(u - \bar{u})k^{-1}A^\dagger \left(A^\dagger + ikB^\dagger\right)^{-1} k && \text{(B.52)}\\
&- 4ik'^{-1} \left(A - iBk'\right)^{-1} Ak'^{-1}uk^{-1}A^\dagger \left(A^\dagger + ikB^\dagger\right)^{-1} k && \text{(B.53)}\\
&= 2ik' \left(A - iBk'\right)^{-1} \Big[Ak'^{-1}(\bar{u} + u)k^{-1} \left(A^\dagger + ikB^\dagger\right) + \left(A - iBk'\right) k'^{-1}(u - \bar{u})k^{-1}A^\dagger && \text{(B.54)}\\
&-2Ak'^{-1}uk^{-1}A^\dagger\Big] \left(A^\dagger + ikB^\dagger\right)^{-1} k && \text{(B.55)}
\end{aligned}$$

with the bracketed term being

$$\frac{1}{2m\Delta\varepsilon} \left[2Ak^{-1} \left(A^\dagger + ikB^\dagger\right) + 2 \left(A - iBk'\right) k'^{-1}A^\dagger - 2Ak'^{-1}(k + k')k^{-1}A^\dagger\right] = 0. \tag{B.56}$$

C Wavefunctions are orthogonal for a complex momentum-matrix

Ignore the proportionality constant and write the wavefunction as

$$\chi_{ab}(x, \varepsilon) = e^{-ik_a^o x}\delta_{ba} + e^{i(k_b^o + ik_b^c)x} S_{ba}(\varepsilon), \quad x \in (0, \infty),\ 1 \le a \le n,\ 1 \le b \le N. \tag{C.1}$$

since we can only insert a wave into open channels. Depending on what channel we're probing, b, we either get a wave returning if b belongs to an open channel, or an exponential decrease if b is a closed channel.

$$\langle \chi_\alpha(\varepsilon') | \chi_\beta(\varepsilon) \rangle = \sum_{j=1}^{N} \int_0^\infty \mathrm{d}x \ \left(e^{ik_\alpha^{o\prime} x}\delta_{\alpha j} + e^{-k_j^{c\prime} x} e^{-ik_j^{o\prime} x} S_{j\alpha}^*(\varepsilon')\right) \left(e^{-ik_\beta^o x}\delta_{\beta j} + e^{-k_j^c x} e^{ik_j^o x} S_{j\beta}(\varepsilon)\right) \tag{C.2}$$

$$\begin{aligned}
\langle \chi_\alpha(\varepsilon') | \chi_\beta(\varepsilon) \rangle = \sum_{j=1}^{N} \int_0^\infty \mathrm{d}x \ \Big(&e^{ix(k_\alpha^{o\prime} - k_\beta^o)}\delta_{\alpha j}\delta_{\beta j} + e^{ix(k_\alpha^{o\prime} + k_j^o)} e^{-k_j^c x}\delta_{\alpha j} S_{j\beta}(\varepsilon)\\
&+ e^{-ix(k_j^{o\prime} + k_\beta^o)} e^{-k_j^{c\prime} x}\delta_{\beta j} S_{j\alpha}^*(\varepsilon') + e^{ix(k_j^o - k_j^{o\prime})} e^{-x(k_j^c + k_j^{c\prime})} S_{j\alpha}^*(\varepsilon') S_{j\beta}(\varepsilon)\Big).
\end{aligned} \tag{C.3}$$

Now, α and β are restricted as

$$1 \le \alpha \le n', \quad 1 \le \beta \le n. \tag{C.4}$$

In the following, we will assume that

$$\varepsilon' > \varepsilon, \quad n' \ge n, \tag{C.5}$$

where the equality $n' = n$ is true when there is at least one intermediate μ_i making $\varepsilon' - \varepsilon < \mu_i - \mu_{i-1}$ (assuming $\mu_1 < \mu_2 < \cdots < \mu_N$).

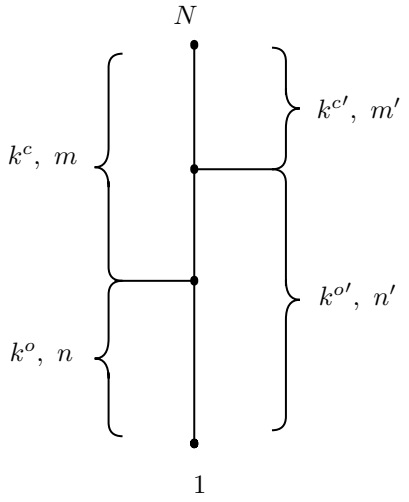


Figure 10: $1 \leq \alpha \leq n'$ and $1 \leq \beta \leq n$. The n, n', m, m' together with k indicate on how many indecies the matrix k have non-zero components. Like k^c has n zeros on the diagonal followed by m non-zero numbers.

We will now calculate the four terms in (C.3), term by term, starting with the first.

Term 1 in (C.3):

$$\sum_{j=1}^{N} \int \mathrm{d}x\, e^{ix(k_\alpha^{o\prime} - k_\beta^o)} \delta_{\alpha j} \delta_{j\beta} = \sum_{j=1}^{N} \delta_{\alpha j} \delta_{j\beta} \left(\pi \delta(k_\alpha^{o\prime} - k_\beta^o) + \frac{i}{k_\alpha^{o\prime} - k_\beta^o} \right) \tag{C.6}$$

$$= \pi \delta_{\alpha\beta} \delta(\varepsilon' - \varepsilon) v_\alpha^o + \delta_{\alpha\beta} \frac{i}{k_\alpha^{o\prime} - k_\alpha^o}. \tag{C.7}$$

with

$$\sum_{j=1}^{N} \delta_{\alpha j} \delta_{j\beta} = \left(\Pi_o' \Pi_o^\top \right)_{\alpha\beta}, \quad \Pi_o' \Pi_o^\top = \begin{pmatrix} \mathbf{1}_n \\ \hline \mathbf{0}_{(n'-n)\times n} \end{pmatrix} \tag{C.8}$$

where $\mathbf{1}_n$ is the $n \times n$ identity matrix and $\mathbf{0}_{(n'-n)\times n}$ is the $(n'-n) \times n$ matrix filled exclusively with zeroes.

Term 2:

$$\sum_{j=1}^{N} \int \mathrm{d}x\, e^{ixk_\alpha^{o\prime}} e^{ixk_j^o} e^{-k_j^c x} \delta_{\alpha j} S_{j\beta}(\varepsilon) = \sum_{j=1}^{n'} \frac{i}{k_\alpha^{o\prime} + k_j^o + ik_j^c} \delta_{\alpha j} S_{j\beta}(\varepsilon) = \frac{i}{k_\alpha^{o\prime} + k_\alpha^o + ik_\alpha^c} S_{\alpha\beta}(\varepsilon) \tag{C.9}$$

Term 3:

$$\sum_{j=1}^{N} \int \mathrm{d}x\, e^{-ixk_j^{o\prime}} e^{-ixk_\beta^o} e^{-k_j^{c\prime} x} \delta_{\beta j} S_{j\alpha}^*(\varepsilon') = \sum_{j=1}^{n} \frac{-i}{k_\beta^o + k_j^{o\prime}} \delta_{\beta j} S_{j\alpha}^*(\varepsilon') = S_{\alpha\beta}^\dagger(\varepsilon') \frac{-i}{k_\beta^o + k_\beta^{o\prime}} \tag{C.10}$$

Term 4:

$$\sum_{j=1}^{N}\int \mathrm{d}x\; e^{ix(k_j^o-k_j^{o\prime})}e^{-x(k_j^c+k_j^{c\prime})}S^*_{j\alpha}(\varepsilon')S_{j\beta}(\varepsilon) \tag{C.11}$$

$$=\sum_{j=1}^{n}S^\dagger_{\alpha j}(\varepsilon')\left[\pi\delta(k_j^{o\prime}-k_j^o)-\frac{i}{k_j^{o\prime}-k_j^o}\right]S_{j\beta}(\varepsilon)+\sum_{j=n+1}^{N}S^\dagger_{\alpha j}(\varepsilon')\frac{-i}{k_j^{o\prime}-i(k_j^{c\prime}+k_j^c)}S_{j\beta}(\varepsilon) \tag{C.12}$$

$$=\pi\delta(\varepsilon'-\varepsilon)\sum_{j=1}^{n}S^\dagger_{\alpha j}(\varepsilon)v_j^oS_{j\beta}(\varepsilon)+\sum_{j=1}^{N}S^\dagger_{\alpha j}(\varepsilon')\frac{-i}{k_j^{o\prime}-k_j^o-i(k_j^{c\prime}+k_j^c)}S_{j\beta}(\varepsilon). \tag{C.13}$$

The matrices $S(\varepsilon)$ and $S^\dagger(\varepsilon')$ written above, are still $N\times n$ and $n'\times N$ respectively. For the wave-functions to be orthogonal we want

$$\langle\chi_\alpha(\varepsilon')|\chi_\beta(\varepsilon)\rangle\propto\delta_{\alpha\beta}\delta(\varepsilon'-\varepsilon) \tag{C.14}$$

meaning, taken from the first term in (C.7) and (C.13) we get

$$\pi\delta(\varepsilon'-\varepsilon)\delta_{\alpha\beta}v_\alpha^o+\pi\delta(\varepsilon'-\varepsilon)\sum_{j=1}^{n}S^\dagger_{\alpha j}(\varepsilon')v_j^oS_{j\beta}(\varepsilon)\overset{!}{\propto}\delta_{\alpha\beta}\delta(\varepsilon'-\varepsilon) \tag{C.15a}$$

$$=\pi\delta(\varepsilon'-\varepsilon)v_\alpha^o\left[\delta_{\alpha\beta}+\sqrt{v_\alpha^o}^{-1}\sum_{j=1}^{N}\sqrt{v_\alpha^o}^{-1}S^\dagger_{\alpha j}(\varepsilon)\sqrt{v_j^o}\sqrt{v_j^o}S_{j\beta}(\varepsilon)\sqrt{v_\beta^o}^{-1}\sqrt{v_\beta^o}\right] \tag{C.15b}$$

$$=\pi\delta(\varepsilon'-\varepsilon)v_\alpha^o\left[\delta_{\alpha\beta}+\sqrt{v_\alpha^o}^{-1}\left(\sqrt{\nu^o}^{-1}S^\dagger(\varepsilon)\sqrt{v^o}\sqrt{v^o}S(\varepsilon)\sqrt{\nu^o}^{-1}\right)_{\alpha\beta}\sqrt{v_\beta^o}\right] \tag{C.15c}$$

$$=\pi\delta(\varepsilon'-\varepsilon)v_\alpha^o\left[\delta_{\alpha\beta}+\sqrt{v_\alpha^o}^{-1}\left(\sqrt{\nu^o}^{-1}S^\dagger(\varepsilon)\Pi_o^\top\sqrt{\nu^o}\sqrt{\nu^o}\Pi_oS(\varepsilon)\sqrt{\nu^o}^{-1}\right)_{\alpha\beta}\sqrt{v_\beta^o}\right] \tag{C.15d}$$

$$=2\pi v_\alpha^o\delta_{\alpha\beta}\delta(\varepsilon'-\varepsilon) \tag{C.15e}$$

since $\left(\hat{S}^\dagger(\varepsilon)\hat{S}(\varepsilon)\right)_{\alpha\beta}=\delta_{\alpha\beta}$. Now we need to show that all the remaining terms that were not proportional to $\delta_{\alpha\beta}\delta(\varepsilon'-\varepsilon)$ vanish. Those remaining terms are called G and are as follows.

$$G_{\alpha\beta}=\delta_{\alpha\beta}\frac{i}{k_\beta^{o\prime}-k_\beta^o}+\frac{i}{k_\alpha^{o\prime}+k_\alpha^o+ik_\alpha^c}S_{\alpha\beta}(\varepsilon)$$
$$-S^\dagger_{\alpha\beta}(\varepsilon')\frac{i}{k_\beta^{o\prime}+k_\beta^o}+\sum_{j=1}^{N}S^\dagger_{\alpha j}(\varepsilon')\frac{i}{k_j^o-k_j^{o\prime}+i(k_j^{c\prime}+k_j^c)}S_{j\beta}(\varepsilon) \tag{C.16}$$

or on matrix form

$$-iG=\Pi_o'K\Pi_o^\top-S^\dagger(\varepsilon')KS(\varepsilon)+\Pi_o'\bar{K}S(\varepsilon)-S^\dagger(\varepsilon')\bar{K}\Pi_o^\top \tag{C.17}$$

with

$$K=\left(-k^o+k^{o\prime}-i(k^{c\prime}+k^c)\right)^{-1}\quad\text{and}\quad\bar{K}=\left(k^o+k^{o\prime}+i(k^{c\prime}+k^c)\right)^{-1} \tag{C.18}$$

$$K=\left(k'^*-k\right)^{-1},\quad\bar{K}=\left(k+k'^*\right)^{-1} \tag{C.19}$$

both being $N \times N$, complex, diagonal and invertible, and * means complex conjugation. We thus need to show that $G_{\alpha\beta} = 0$. To begin, we write

$$K = (k'^* + k)/2m\Delta\varepsilon, \quad \bar{K} = (k'^* - k)/2m\Delta\varepsilon. \tag{C.20}$$

and by letting

$$S(\varepsilon) = \Pi_o^\top + iT(\varepsilon), \tag{C.21}$$

we find

$$-2imG\Delta\varepsilon = -2i\Pi_o' kT(\varepsilon) + 2iT^\dagger(\varepsilon')k'^*\Pi_o^\top - T^\dagger(\varepsilon')(k'^* + k)T(\varepsilon). \tag{C.22}$$

$$\hat{S}(\varepsilon) = 1 + i\hat{T}(\varepsilon) \tag{C.23}$$

From (D.10) we know that

$$\hat{T}_{A,B,\kappa^o}(\varepsilon) = \hat{T}^\top_{iA^*,-iB^*,-\kappa^o}(\varepsilon), \tag{C.24}$$

with $\hat{T}_{A,B,\kappa^o}(\varepsilon) = \hat{T}(\varepsilon)$ and the notation $\hat{T}_{iA^*,-iB^*,-\kappa^o}(\varepsilon)$ means $\hat{T}_{A,B,\kappa^o}(\varepsilon)$ with $A \to iA^*$, $B \to -iB^*$ and $\kappa^o \to -\kappa^o$ and $\sqrt{-\kappa^o} = i\sqrt{\kappa^o}$ and $\sqrt{-\kappa^o}^{-1} = -i\sqrt{\kappa^o}^{-1}$. Following the same procedure as (B.33) we find the two version of $\hat{T}$ from (C.24)

$$\hat{T}(\varepsilon) = 2i\left(\tilde{A}\sqrt{\kappa^o}^{-1} + i\tilde{B}\sqrt{\kappa^o}\right)^{-1}\tilde{A}\sqrt{\kappa^o}^{-1} \tag{C.25a}$$

$$= 2i\sqrt{\kappa^o}^{-1}\tilde{A}^\dagger\left(\sqrt{\kappa^o}^{-1}\tilde{A}^\dagger + i\sqrt{\kappa^o}\tilde{B}^\dagger\right)^{-1} \tag{C.25b}$$

$$\hat{T}^\dagger(\varepsilon') = -2i\left(\tilde{A}'\sqrt{\kappa^{o\prime}}^{-1} - i\tilde{B}'\sqrt{\kappa^{o\prime}}\right)^{-1}\tilde{A}'\sqrt{\kappa^{o\prime}}^{-1} \tag{C.25c}$$

$$= -2i\sqrt{\kappa^{o\prime}}^{-1}\tilde{A}'^\dagger\left(\sqrt{\kappa^{o\prime}}^{-1}\tilde{A}'^\dagger - i\sqrt{\kappa^{o\prime}}\tilde{B}'^\dagger\right)^{-1}, \tag{C.25d}$$

and by (C.21):

$$\hat{T}(\varepsilon) = \sqrt{\kappa^o}\Pi_o T(\varepsilon)\sqrt{\kappa^o}^{-1} \tag{C.26}$$

$$\hat{T}^\dagger(\varepsilon') = \sqrt{\kappa^{o\prime}}^{-1}T^\dagger(\varepsilon')\Pi_o'^\top\sqrt{\kappa^{o\prime}} \tag{C.27}$$

but since Π_o does not have a left inverse (and $\Pi_o^\top$ a right), an explicit expression for T is not available, although we can guess and check solutions, such that by the above transformation, satisfy (C.25). So, drawing inspiration from the open scattering matrix formulation, we set

$$T(\varepsilon) = 2ik^{-1}A^\dagger\left(A^\dagger + ikB^\dagger\right)^{-1}k\Pi_o^\top \tag{C.28}$$

$$T^\dagger(\varepsilon') = -2i\Pi_o' k'^*\left(A - iBk'^*\right)^{-1}A(k'^*)^{-1} \tag{C.29}$$

By inserting the identities

$$\mathbf{1}_N = k'^*\left(A - iBk'^*\right)^{-1}\left(A - iBk'^*\right)(k'^*)^{-1} \tag{C.30a}$$

$$\mathbf{1}_N = k^{-1}\left(A^\dagger + ikB^\dagger\right)\left(A^\dagger + ikB^\dagger\right)^{-1}k \tag{C.30b}$$

appropriately, we find

$$-2imG\Delta\varepsilon = 4\Pi_o' k'^* \left(A - iBk'^*\right)^{-1} \Big[(A - iBk'^*)(k'^*)^{-1}kk^{-1}A^\dagger \tag{C.31}$$

$$+ A(k'^*)^{-1}k'^*k^{-1}\left(A^\dagger + ikB^\dagger\right) - Ak'^{*-1}(k'^* + k)k^{-1}A^\dagger\Big]\left(A^\dagger + ikB^\dagger\right)^{-1} k\Pi_o^\top$$

$$= 0. \tag{C.32}$$

D Unitarity of the scattering matrix for a complex momentum-maitrx

We will show that $\hat{S}$ is unitary by following the exact same procedure as done in (B.20) to (B.26), by first defining

$$\tilde{A} = A\Pi_o^\top, \quad \tilde{B} = B\Pi_o^\top \tag{D.1}$$

We now miss the important self-adjointness of $AB^\dagger$ as $\tilde{A}\tilde{B}^\dagger = AP_oB^\dagger$ is not self-adjoint, but $i(\tilde{A}\tilde{B}^\dagger - \tilde{B}\tilde{A}^\dagger)$ is. Π_o has a right inverse: $\Pi_o^\top$, but not a left inverse from. So

$$\Pi_o S(\varepsilon) = -\left(A\Pi_o^\top + iB\Pi_o^\top\kappa^o - B\Pi_c^\top\kappa^c\Pi_c\Pi_o^\top\right)^{-1}\left(A\Pi_o^\top - iB\Pi_o^\top\kappa^o\right) \tag{D.2}$$

$$= -\left(\tilde{A} + i\tilde{B}\kappa^o\right)^{-1}\left(\tilde{A} - i\tilde{B}\kappa^o\right) \tag{D.3}$$

$$\hat{S}(\varepsilon) = -\left(\tilde{A}\sqrt{\kappa^o}^{-1} + i\tilde{B}\sqrt{\kappa^o}\right)^{-1}\left(\tilde{A}\sqrt{\kappa^o}^{-1} - i\tilde{B}\sqrt{\kappa^o}\right). \tag{D.4}$$

$$\hat{S}(\varepsilon) = -\left(\sqrt{\kappa^o}^{-1}\tilde{A}^\dagger - i\sqrt{\kappa^o}\tilde{B}^\dagger\right)\left[\tilde{A}(\kappa^o)^{-1}\tilde{A}^\dagger + i\tilde{B}\tilde{A}^\dagger - i\tilde{A}\tilde{B}^\dagger + \tilde{B}\kappa^o\tilde{B}^\dagger\right]^{-1}\left(\tilde{A}\sqrt{\kappa^o}^{-1} - i\tilde{B}\sqrt{\kappa^o}\right) \tag{D.5}$$

$$\hat{S}^\dagger(\varepsilon) = -\left(\sqrt{\kappa^o}^{-1}\tilde{A}^\dagger + i\sqrt{\kappa^o}\tilde{B}^\dagger\right)\left[\tilde{A}(\kappa^o)^{-1}\tilde{A}^\dagger + i\tilde{B}\tilde{A}^\dagger - i\tilde{A}\tilde{B}^\dagger + \tilde{B}\kappa^o\tilde{B}^\dagger\right]^{-1}\left(\tilde{A}\sqrt{\kappa^o}^{-1} + i\tilde{B}\sqrt{\kappa^o}\right) \tag{D.6}$$

$$\hat{S}^{-1}(\varepsilon) = -\left(\tilde{A}\sqrt{\kappa^o}^{-1} - i\tilde{B}\sqrt{\kappa^o}\right)^{-1}\left(\tilde{A}\sqrt{\kappa^o}^{-1} + i\tilde{B}\sqrt{\kappa^o}\right) \tag{D.7}$$

$$= -\left(\sqrt{\kappa^o}^{-1}\tilde{A}^\dagger + i\sqrt{\kappa^o}\tilde{B}^\dagger\right)\left[\tilde{A}(\kappa^o)^{-1}\tilde{A}^\dagger + i\tilde{B}\tilde{A}^\dagger - i\tilde{A}\tilde{B}^\dagger + \tilde{B}\kappa^o\tilde{B}^\dagger\right]^{-1}\left(\tilde{A}\sqrt{\kappa^o}^{-1} + i\tilde{B}\sqrt{\kappa^o}\right) \tag{D.8}$$

$$= \hat{S}^\dagger(\varepsilon). \tag{D.9}$$

So $\hat{S}(\varepsilon)$ is unitary. This is without proving the existence of the different inverses, which may prove troublesome as $\tilde{A}\tilde{B}^\dagger$ is not self-adjoint. From (D.5) one can confirm

$$\hat{S}_{A,B,\kappa^o}(\varepsilon) = \hat{S}^\top_{iA^*,-iB^*,-\kappa^o}(\varepsilon), \tag{D.10}$$

with $\sqrt{-\kappa^o} = i\sqrt{\kappa^o}$ and $\sqrt{-\kappa^o}^{-1} = -i\sqrt{\kappa^o}$

E Delta function wavefunctions are orthogonal

For orthogonality, equation (B.29), we want $f = 0$ for

$$f = u + \bar{u}\hat{S}(\varepsilon) - \hat{S}^\dagger(\varepsilon')\bar{u} - \hat{S}^\dagger(\varepsilon')u\hat{S}(\varepsilon) \tag{E.1}$$

$$= u\left(1 - \hat{S}^\dagger(\varepsilon')\hat{S}(\varepsilon)\right) + \bar{u}\left(\hat{S}(\varepsilon) - \hat{S}^\dagger(\varepsilon')\right) \tag{E.2}$$

$$= u\left(1 - e^{-i(\theta-\theta')}\right) + \bar{u}\left(e^{-i\theta} - e^{i\theta'}\right) \tag{E.3}$$

$$= u\left(1 - e^{-i(\theta-\theta')}\right) - 2i\bar{u}e^{-i(\theta-\theta')/2}\sin\frac{\theta+\theta'}{2}. \tag{E.4}$$

with $\theta = \theta(\varepsilon)$, $\theta' = \theta(\varepsilon')$ and

$$u = (k - k')^{-1}, \quad \bar{u} = (k + k')^{-1}. \tag{E.5}$$

First define

$$\mathcal{D} = \left(BB^\dagger k - AA^\dagger k^{-1}\right)\left(BB^\dagger k' - AA^\dagger k'^{-1}\right) \tag{E.6}$$

and

$$g = \frac{-AB^\dagger}{BB^\dagger k - AA^\dagger k^{-1}}, \quad g' = \frac{-AB^\dagger}{BB^\dagger k' - AA^\dagger k'^{-1}} \tag{E.7}$$

so that

$$\theta = \tan^{-1} g, \quad \theta' = \tan^{-1} g'. \tag{E.8}$$

Thus

$$f = u(1 - \cos\theta\cos\theta' - \sin\theta\sin\theta') + \bar{u}(\cos\theta - \cos\theta') + i\left[u(\sin\theta\cos\theta' - \cos\theta\sin\theta') - \bar{u}(\sin\theta + \sin\theta')\right]. \tag{E.9}$$

$$\mathrm{Re}\{f\} = \frac{1}{\sqrt{1+g^2}\sqrt{1+g'^2}}\left[u\left(\sqrt{1+g^2}\sqrt{1+g'^2} - 1 - gg'\right) + \bar{u}\left(\sqrt{1+g'^2} - \sqrt{1+g^2}\right)\right] \tag{E.10}$$

$$= \frac{1}{\sqrt{1+g^2}\sqrt{1+g'^2}}\left[-u\left(\frac{-2BB^\dagger AA^\dagger(kk'^{-1} + k'k^{-1}) + 4A^2B^{\dagger 2}}{\mathcal{D}}\right)\right. \tag{E.11}$$

$$\left.\bar{u}\left(\frac{2AA^\dagger BB^\dagger(kk'^{-1} - k'k^{-1})}{\mathcal{D}}\right)\right]$$

$$= \frac{1}{\sqrt{1+g^2}\sqrt{1+g'^2}}\left[-\frac{k-k'}{kk'}\frac{2AA^\dagger BB^\dagger}{\mathcal{D}} + \frac{k-k'}{kk'}\frac{2AA^\dagger BB^\dagger}{\mathcal{D}}\right] = 0 \tag{E.12}$$

where we extensively have used that A and B are diagonal, and $AB^\dagger$ is self-adjoint.

$$\mathrm{Im}\{f\} = \frac{1}{\sqrt{1+g^2}\sqrt{1+g'^2}}\left[u(g - g') + \bar{u}\left(\sqrt{1+g'^2}g + \sqrt{1+g^2}g'\right)\right] \tag{E.13}$$

$$= \frac{1}{\sqrt{1+g^2}\sqrt{1+g'^2}}\left[-2uAB^\dagger\frac{BB^\dagger(k'-k) + AA^\dagger(k^{-1} - k'^{-1})}{\mathcal{D}}\right. \tag{E.14}$$

$$\left.-2\bar{u}AB^\dagger\frac{AA^\dagger(k'^{-1} + k^{-1}) + BB^\dagger(k+k')}{\mathcal{D}}\right]$$

$$= 0. \tag{E.15}$$

So we conclude that in the simplest situation, when A and B are diagonal, corresponding to a δ potential at the vertex, the wavefunctions are orthogonal.

F Kirchhoff's law for conductance figures

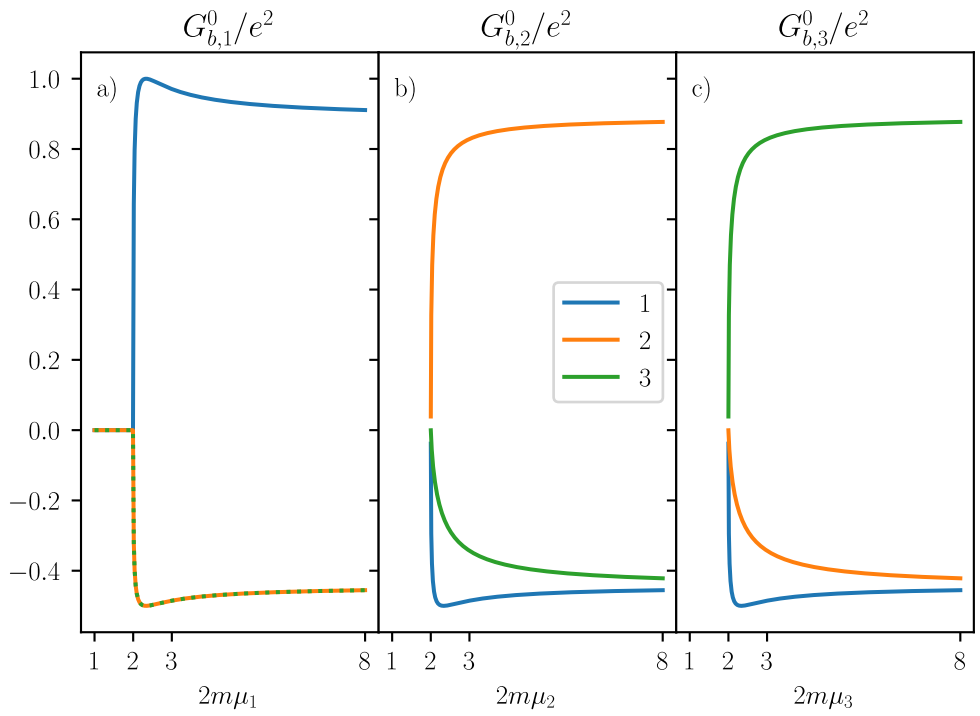
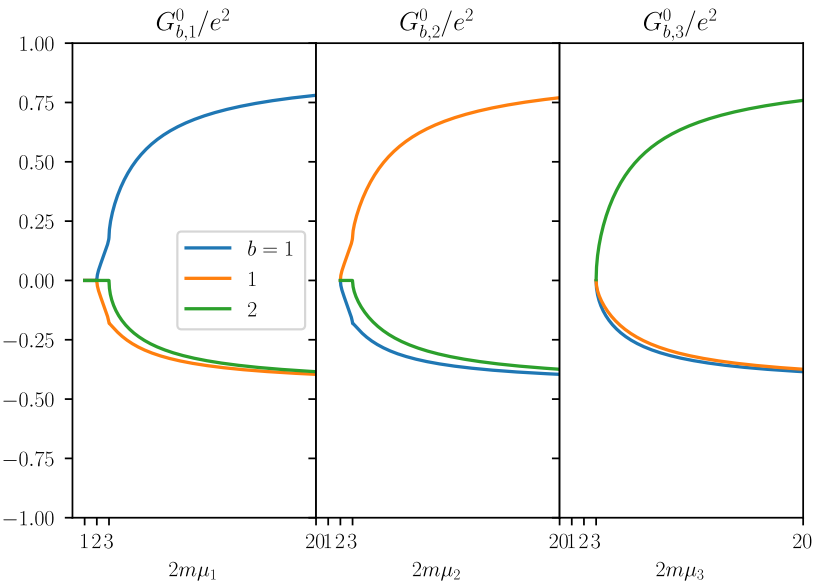
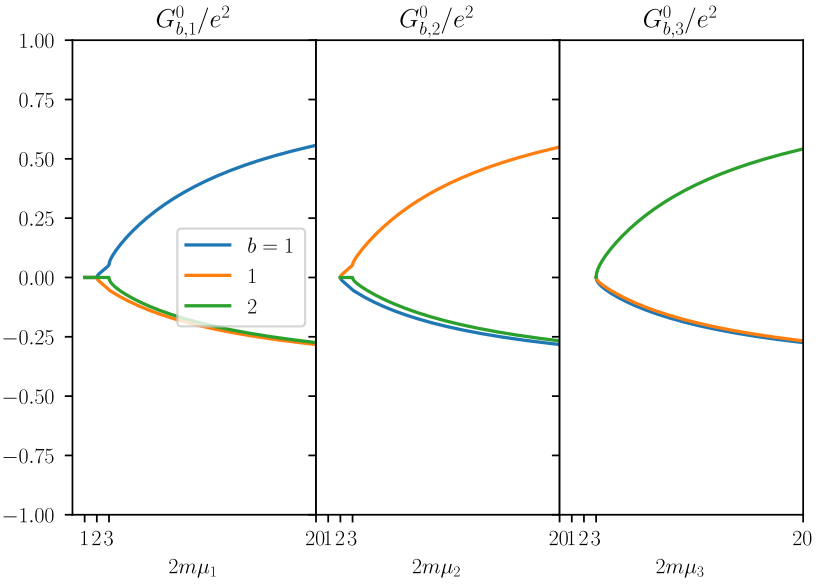


Figure 11: Conductance at zero temperature, with induced potentials given by $2mu = \{1, 2, 2\}$, $\alpha = 0$.



(a) $\alpha = 5$



(b) $\alpha = 10$

Figure 12: Induced potentials $2mu = \{1, 2, 3\}$. As α increase, any conductance decrease, i.e. each lead becomes isolated.

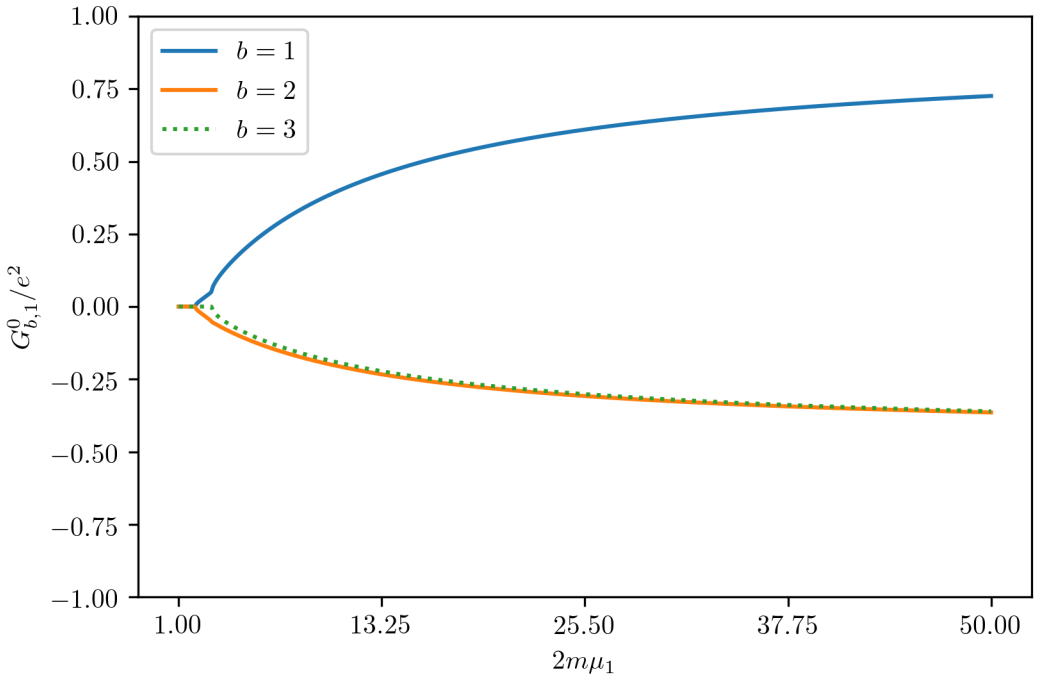


Figure 13: Here $\alpha = 10$, and $2mu = \{1, 2, 3\}$)

G Observables derivations

The electric current:

$$\langle J_b(x)\rangle = \frac{i}{2m}\iint \frac{\mathrm{d}\varepsilon\,\mathrm{d}\varepsilon'}{2\pi}\sum_{a',a}\langle c^\dagger_{a'}(\varepsilon')c_a(\varepsilon)\rangle\left[\chi^*_{a'b}(x,\varepsilon')\partial_x\chi_{ab}(x,\varepsilon) - \partial_x\chi^*_{a'b}(x,\varepsilon')\,\chi_{ab}(x,\varepsilon)\right] \tag{G.1}$$

$$= \frac{i}{2m}\int \mathrm{d}\varepsilon \sum_a f_a[\chi^*_{ab}(x,\varepsilon)\partial_x\chi_{ab}(x,\varepsilon) - c.c.] \tag{G.2}$$

$$= \frac{i}{2m}\int \mathrm{d}\varepsilon \sum_a \frac{f_a}{v^o_a}\Big[\left(e^{ik^o_a x}\delta_{ab} + e^{-i(k^o_b - ik^c_b)x}S^*_{ba}(\varepsilon)\right) \tag{G.3}$$

$$\times\left(-ik^o_a e^{-ik^o_a x}\delta_{ab} + i(k^o_b + ik^c_b)e^{i(k^o_b+ik^c_b)x}S_{ba}(\varepsilon)\right) - c.c.\Big]$$

$$= \frac{i}{2m}\sum_{\text{all } a}\int_{\mu_a}^{\infty}\mathrm{d}\varepsilon\frac{f_a}{v^o_a}\Big[-2ik^o_a\delta^2_{ab} + i\delta_{ab}S_{ba}(\varepsilon)\left((k^o_b + ik^c_b)e^{ik^o_a x}e^{i(k^o_b+k^c_b)x} - k^o_a e^{ik^o_a x}e^{i(k^o_b+ik^c_b)x}\right)$$

$$- i\delta_{ab}S^*_{ba}(\varepsilon)\left(k^o_a e^{-ik^o_a x}e^{-ik^o_b - ik^c_b x} - (k^o_b - ik^c_b)e^{-ik^o_a x}e^{-i(k^o_b - ik^c_b)x}\right) + 2ie^{-2k^c_b x}k^o_b|S_{ba}(\varepsilon)|^2\Big]$$

$$= \int_{\mu_b}^{\infty}\mathrm{d}\varepsilon\; f_b(\varepsilon) - \int_0^{\infty}\mathrm{d}\varepsilon\; e^{-2k^c_b x}\sum_{a\in\mathcal{O}(\varepsilon)} f_a(\varepsilon)\frac{k^o_b}{k^o_a}|S_{ba}(\varepsilon)|^2 \tag{G.4}$$

$$\langle J_b(x)\rangle = \int_{\mu_b}^{\infty}\mathrm{d}\varepsilon\sum_{a\in\mathcal{O}(\varepsilon)}\left[f_b(\varepsilon) - f_a(\varepsilon)\right]|\hat{S}_{ba}(\varepsilon)|^2 \tag{G.5}$$

$$= \int_{\mu_b}^{\infty}\mathrm{d}\varepsilon\sum_{a\in\mathcal{O}(\varepsilon)}[\delta_{ab} - |\hat{S}_{ab}(\varepsilon)|^2]f_a(\varepsilon) \tag{G.6}$$

The particle density:

$$\langle \rho_b(x) \rangle = \iint \frac{\mathrm{d}\varepsilon \, \mathrm{d}\varepsilon'}{2\pi} \sum_{a',a} \langle c^\dagger_{a'}(\varepsilon') c_a(\varepsilon) \rangle \chi^*_{a'b}(x,\varepsilon') \chi_{ab}(x,\varepsilon) \tag{G.7}$$

$$= \int_0^\infty \mathrm{d}\varepsilon \sum_a f_a |\chi_{ab}(x,\varepsilon)|^2 \tag{G.8}$$

$$\langle \rho_{b,\mathcal{O}}(x) \rangle = \int_{\mu_b}^\infty \mathrm{d}\varepsilon \sum_{a \in \mathcal{O}(\varepsilon)} f_a |\chi_{ab}(x,\varepsilon)|^2 \tag{G.9}$$

$$= \int_{\mu_b}^\infty \mathrm{d}\varepsilon \sum_{\text{all } a} \frac{f_a(\varepsilon)\theta(\varepsilon - \mu_a)}{v_a^o} \left(\delta_{ab}^2 + 2\delta_{ab} \operatorname{Re}\left\{ e^{ik_a^o x} e^{i(k_b^o + ik_b^c)x} S_{ba}(\varepsilon) \right\} + e^{-2k_b^c x} |S_{ba}(\varepsilon)|^2 \right) \tag{G.10}$$

$$= \int_{\mu_b}^\infty \mathrm{d}\varepsilon \left[\frac{f_b(\varepsilon)}{v_b^o} \left(1 + 2 \operatorname{Re}\left\{ e^{2ik_b^o x} S_{bb}(\varepsilon) \right\} \right) + \sum_{a \in \mathcal{O}(\varepsilon)} \frac{f_a(\varepsilon)}{v_a^o} |S_{ba}(\varepsilon)|^2 \right] \tag{G.11}$$

$$\langle \rho_{b,\mathcal{C}}(x) \rangle = \int_0^{\mu_b} \sum_{a \in \mathcal{O}(\varepsilon)} f_a |\chi_{ab}(x,\varepsilon)|^2 \tag{G.12}$$

$$= \int_0^{\mu_b} \mathrm{d}\varepsilon \; e^{-2k_b^c x} \sum_{a \in \mathcal{O}(\varepsilon)} \frac{f_a(\varepsilon)}{v_a^o} |S_{ba}(\varepsilon)|^2. \tag{G.13}$$

$$\langle \rho_b(x) \rangle = \int_{\mu_b}^\infty \mathrm{d}\varepsilon \left[\frac{f_b(\varepsilon)}{v_b^o} \left(1 + 2 \operatorname{Re}\left\{ e^{2ik_b^o x} S_{bb}(\varepsilon) \right\} \right) + \sum_{a \in \mathcal{O}(\varepsilon)} \frac{f_a(\varepsilon)}{v_a^o} |S_{ba}(\varepsilon)|^2 \right] + \int_0^{\mu_b} \mathrm{d}\varepsilon \; e^{-2k_b^c x} \sum_{a \in \mathcal{O}(\varepsilon)} \frac{f_a(\varepsilon)}{v_a^o} |S_{ba}(\varepsilon)|^2 \tag{G.14}$$

$$\langle \rho_b(x) \rangle = \int_{\mu_b}^\infty \mathrm{d}\varepsilon \frac{f_b(\varepsilon)}{v_b^o} \left(1 + 2 \operatorname{Re}\left\{ e^{2ik_b^o x} S_{bb}(\varepsilon) \right\} \right) + \int_0^\infty \mathrm{d}\varepsilon \; e^{-2k_b^c x} \sum_{a \in \mathcal{O}(\varepsilon)} \frac{f_a(\varepsilon)}{v_a^o} |S_{ba}(\varepsilon)|^2 \tag{G.15}$$

k_b^c is only defined if $\mu_b > \varepsilon$, else return 0. At non-zero temperature there will always be a non-zero number of particles in each lead.