The conductivity of Kitaev's chain

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Chapter 1

Introduction to Majorana fermions

A Majorana fermion is a theoretically hypothesised particle that has no anti-matter counterpart; instead, it is its own anti-particle. This original idea comes from the field of high energy physics where it still inspires theoretical work on neutrino physics, dark matter and supersymmetry. Nowadays, thanks to theoretical proposals of condensed matter physics and experimental achievements in nano-materials, several systems rise as candidates for the physical realisation of Majorana fermions. Majorana fermions in condensed matter systems show an exotic particle statistics behaviour which classifies them as non-Abelian anyons. The implementation of a quantum device able to accommodate such exotic particles envisages of fault tolerant quantum computation.

1.1 The original hypothesis

In 1928 Paul Dirac published his seminal work "The Quantum Theory of the Electron" [1], suggesting a governing equation of motion for the free relativistic electron. Until that time, the Klein-Gordon equation was understood as the governing one for relativistic particles, even though it posed problems to physics since it led to negative probability densities.

Driven by a desire to liberate quantum theory from the negative probability densities of the Klein-Gordon equation, Dirac suggested an equation linear in its time derivative ∂_t, while it remained Lorentz invariant. Setting those two requirements ab initio, the equation uncovered had an unexpectedly enriching influence to physics. At once, the quantum number of spin $1/2$ - naturally incorporated in Dirac's equation - was explained, while the existence of anti-matter was proposed. Dirac interpreted the negative energy solutions of an electron as positive energy solutions of an opposite charged particle, the positron. The explanative power of physics for our material world faced the rise of anti-matter!

Apart from the poetic metaphors, Dirac's equation does bear aesthetic beauty due to its mathematical elegance. It allows solutions that are complex valued; given that electrons are charged particles. This is a desirable consequence since a spinor ψ describing an electron, will have a counterpart conjugate spinor $\psi_c = C\psi^*$, that describes its anti-particle, the positron. Pause; what if there is a solution of Dirac's equation involving a purely real valued spinor field $\phi = \phi_c$? Wouldn't this mean that the particle described would on the same time be it's own anti-particle? Deliberately, the answer is "Yes!" and the particle described by such a field is nowadays called a Majorana Fermion.

Ettore Majorana, in his 1937 paper [2], suggested a purely imaginary representation for the Dirac $\gamma-$matrices, which in terms of Pauli matrices σ_i, check app.A, reads as

$$\gamma_0 = \sigma_2 \otimes \sigma_1\,, \quad \gamma_1 = i\sigma_1 \otimes \hat{1}_2, \quad \gamma_2 = i\sigma_3 \otimes \hat{1}_2, \quad \gamma_3 = i\sigma_2 \otimes \sigma_2. \tag{1.1}$$

The representation is such that the anti-commutation relation of the Clifford algebra is preserved, namely

$$\{\gamma_\mu, \gamma_\nu\} = \gamma_\mu\gamma_\nu + \gamma_\nu\gamma_\mu = 2\eta_{\mu\nu} \tag{1.2}$$

is satisfied, where $\eta_{\mu\nu}$ is Minkowski's metric with signature $(+,-,-,-,)$. But now Dirac's equation

$$(i\gamma^\mu\partial_\mu - m)\,\phi = 0\,, \tag{1.3}$$

has a real valued solution ϕ; note how the term $i\gamma^\mu$ has been turned real in Majorana's representation! The field ϕ has preserved its spin $1/2$ nature while describing a fermion which is at the same time an anti-particle. As Hermann Weyl refined Dirac's work for massless particles in 1929 [3], showing how in that case helicity coincides with chirality, Ettore Majorana distilled an equation that makes particles and anti-particles coincide.

Since his original publication several attempts for the physical realisation of Majorana's theoretical proposal have been done mainly in high energy physics. The neutrino is among the most promising particles that could be described as a Majorana fermion while contemporary candidates include supersymmetric partinos and dark matter.

1.2 Under the kaleidoscope of Condensed Matter

Another candidate, for the physical realisation of Majorana's idea comes from a traditionally "down to Earth" physics area, condensed matter physics. The picture in this discipline is different than the one expected, since condensed matter systems lack Lorentz invariance while their constituents - no matter how exotic a material could be - are electrons, ions and photons as interaction's mediators.

Firstly, the requirement for a non-Lorentz invariant theory drives physics away from Dirac's equation and make Majorana's mathematically elegant theory of the imaginary representation of γ-matrices and the real valued scalar field ϕ, literally dull. There nevertheless still *is* room for Majorana's idea in solid state physics; just recall a bit of theory about superconductivity. The basic constituent - the Cooper pairs - responsible for superconductivity, are bound states of two electrons which violate Pauli's exclusion principle forming a Bose-Einstein condensate. Under this superconducting phase there are fermionic states which couple electrons with holes of the Fermi sea.

In second quantization language, an operator $c^\dagger_{k,\sigma}$ creates an electron of momentum k above the Fermi level and spin σ, while it's Hermitian conjugate operator $c_{k,\sigma}$ annihilates it or it creates a physically distinct state, a hole, which behaves like the anti-particle of the corresponding valence electron. A parti-hole excitation above the ground state is mathematically represented by linear combinations of the form $d_k = a\,c^\dagger_{k,\uparrow} + b^*\,c_{-k,\downarrow}$, in the so-called Bogoliubov-Valatin formalism. Now, what if there were states that turned to themselves by Hermitian conjugation? Wouldn't this mean that the contrast of particles and anti-particles has been evaporated, as Majorana suggested?

Obviously, the Hermitian conjugate of a parti-hole excitation in the form of the abovementioned one, namely $d^\dagger_k = a^*\,c^\dagger_{k,\uparrow} + b\,c_{-k,\downarrow}$, is distinct as spin ruins our dream for a Majorana

particle even for the case of $|a| = |b|$ and $k = 0$. On the other hand, it sheds light to a plausible suggestion; spinless superconductivity could "do the trick". A superconducting material where Cooper pairing is done in a p-wave fashion is effectively spinless and quasiparticle excitations of the special form $f_k = f_k^\dagger = a c^\dagger + a^* c$ are identical to their conjugates. This p-wave superconductor is a promising playground for Majorana's exotic particles and has revamped contemporary theoretical research about his old idea.

1.3 Praying for mathematical formalism

Under the promise of p-wave superconductivity, through a heuristic approach we can formally define Majorana operators γ_a as

$$\gamma_{2i-1} = c_i^\dagger + c_i\,, \tag{1.4a}$$

$$\gamma_{2i} = i(c_i^\dagger - c_i)\,, \tag{1.4b}$$

in terms of ordinary creation/annihilation operators $c_i^\dagger / c_i$ for spinless fermions. Those satisfy the canonical anti-commutation relations

$$\{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0 \quad \& \quad \{c_i, c_j^\dagger\} = \delta_{ij}\,, \tag{1.5}$$

where the indices $i, j \in \mathbb{Z}$ serve as labels of the fermions, e.g. in an optical lattice, those indices label the sites. Afterwards, we are able to confirm that the Majorana operators γ_k satisfy the relation

$$\gamma_a = \gamma_a^\dagger\,, \tag{1.6}$$

while obeying the anti-commutation relation of the Clifford algebra

$$\{\gamma_a, \gamma_b\} = 2\delta_{ab} \Leftrightarrow \gamma_a\gamma_b + \gamma_b\gamma_a = 2\delta_{ab}\,, \tag{1.7}$$

where $a, b \in \mathbb{Z}$. Inverting eq.(1.4) shows that our proposal may be interpreted as the "splitting" of a fermion into a real and an imaginary part; the fermionic creation/annihilation operators $c_i^\dagger / c_i$ are written as

$$c_i^\dagger = \frac{1}{2}(\gamma_{2i-1} - i\gamma_{2i})\,, \tag{1.8a}$$

$$c_i = \frac{1}{2}(\gamma_{2i-1} + i\gamma_{2i})\,, \tag{1.8b}$$

while the Pauli principle does not apply for the Majorana operators, since

$$\gamma_a\gamma_a^\dagger = \gamma_a^2 = 1 \tag{1.9}$$

according to the anti-commutaton relation of the Clifford algebra suggested in eq.(1.7). Recall that for ordinary fermions $c_i^2 = (c_i^\dagger)^2 = 0$, whereas for Majorana γ-operators we encounter an opposite situation; acting twice on a state takes us back to the same state! Consequently, there can be no occupancy number operator defined for Majorana fermions; given the usual definition $n_i = c_i^\dagger c_i = \frac{1}{2}(1 + i\gamma_{2i-1}\gamma_{2i})$ while using the same definition for Majorana operators, i.e. $m_a = \gamma_a^\dagger\gamma_a$, always results in an occupancy number equal to 1, since $\gamma_a^\dagger\gamma_a = 1$.

1.4 A dialogue on the character of Majoranas

– Just a moment! We are going too far... As long as there is no Pauli exclusion principle we cannot call our Majoranas "fermions"...

– Sure! Maybe the term “fermion” is a little abusive but my operators do satisfy an anti-commutation rule which is fermionic, look at eq.(1.7)! I don’t even have a commutator for them that resembles to bosons...

– Then we should investigate the exchange statistics in order to deliver a clear verdict about their nature...

– Fair... Let us assume a quasi-fermion state $|\Psi_0\rangle$ able to be turn into a ground state while it accommodates a Majorana γ_a, e.g. in the form $\gamma_a|\Psi_0\rangle$. Acting on it with the another Majorana operator γ_b, creates the state $\gamma_b\gamma_a|\Psi_0\rangle = -\gamma_a\gamma_b|\Psi_0\rangle$ while returning to the ground state means $\gamma_b\gamma_b\gamma_a|\Psi_0\rangle = \gamma_b^2\gamma_a|\Psi_0\rangle = \gamma_a|\Psi_0\rangle$. Both properties are consistent for fermions.

See... Using the commutation relations and properties for the Majorana operators given, plus an arbitrary state accommodative of Majoranas $\gamma_a|\Psi_0\rangle$, we confirm that Majoranas are fermions! Or if you prefer... anyons, whose phase factor is π. Every time you exchange two of them they pick a multiplication factor $e^{i\pi} = -1$.

– Hmmm... What if the ground state is not unique. Assume a degeneracy on it... Then an exchange may transform one ground state $|\Psi_0\rangle$ into a different one $|\Psi_1\rangle$. The exchange should be represented by a unitary matrix, such that a transformation from one ground state to another consists of a set of consecutive exchanges. This results in a product of unitary matrices. But matrix products are non-commutative, hence...

– Εὕρηκα! Εὕρηκα! The Majoranas are non-Abelian anyons!

1.5 A promising qubit?

For non-Abelian statistics the existence of a degenerate ground state separated from all other excited states is of major importance, as we have discussed in the previous paragraph. Letting the degeneracy be two-fold, we represent the ground states as $|0\rangle$ and $|1\rangle$ in Dirac’s bracket notation. In the meanwhile - under a surrealist’s inspiration - we become reminiscent of the basic unit of computing, the so-called binary digit or bit which has also a two-fold nature. For systems with degenerate states, I call $|0\rangle$ and $|1\rangle$ qubits - quantum binary digits - and dream of quantum processes that represent the act of computation.

The main obstacle for a quantum computation lies in the heart of quantum mechanics. During a quantum process our qubit states may couple with other excited states of the system causing decoherence and practically ruining any information that could be encoded in the qubits. So, given a sufficient separation between the qubit states and the excited states, in energy, allows us to preserve the state of a qubit for a time interval that is sufficient for a quantum computation.

Given such an energy gap the effective Schrödinger equation for a qubit state $|a\rangle$ is

$$\frac{d}{dt}|a\rangle = -iH_{qubit}|a\rangle. \tag{1.10}$$

This enables us to approximate the time interval Δt allowed for calculations to take place. Or dream of a vanishing qubit hamiltonian, $H_{qubit} = 0$, which will give us the privilege of an infinite time interval, $\Delta t \to \infty$.

In the subsequent chapters, we will see how the non-Abelian character of Majorana fermions arrises and how their existence require a sufficient energy gap of a two-fold degenerate ground state. Surprisingly we will show that this ground state - where Majorana fermions are present - lies at the zero-point of the energy spectrum suggesting them as ideal candidates for encoding quantum information.

1.6 Setting goals

In the upcoming chapters our purpose is to convince the reader that Majorana's idea is alive, in a way that there is promising ground for implementation in condensed matter systems. We will show how a $1D$ lattice of spinless fermions can host Majorana fermions which are spatially separated while they correspond to a degenerate zero-energy mode of the spectrum. The host is known in the literature as Kitaev's chain and it is a tight-binding model of a p-wave superconductor.

Starting from Schrödinger's equation of first quantisation we will sketch the passage to second quantization, which "talks" about condensed matter systems intuitively. Posing justifiable restrictions to generality will lead us to the Hamiltonian of Kitaev's model, which is in a second quantised form. Then calculating the bulk spectrum's dispersion relations will be the next step which will show two different regimes for the superconducting model, a trivial one and topological.

This topological superconductor that Kitaev's model encompasses, is of special interest since the Majorana fermions exist within that phase. They appear spatially separated, at the edges of the $1D$ chain for zero-energy cost and create the degenerate ground state that non-Abelian statistics require. The reader will be guided through the calculation of this ground state, firstly for a 2-site lattice and later for the general case of the N-site one.

Having established an understanding for the properties of Kitaev's chain and set the limits within Majorana fermions appear, we will turn to what the title of this thesis suggests. The conductivity of Kitaev's chain is a physical quantity of particular interest since it could serve as an experimental signature among the different phases of the system. No simpler setting than coupling the system to heat baths of fermions with different chemical potentials $\mu_{L/R}$; this will induce a current though the $1D$ lattice. But, since a current is a non-equilibrium quantity there is no other choice to our method than using non-equilibrium statistical physics.

The heat baths or fermionic reservoirs will be justifiably treated as sources of noise for Kitaev's chain and we will mount on Langevin dynamics. Then using non-equlibrium Green's functions we will show the zero-temperature spectral function and finally the conductivity of the Kitaev's chain in the trivial and the topological phase.

Chapter 2

A host for Majorana's Fermions

In 2001, Alexei Kitaev proposed a toy model of this nature and showed how a $1D$ quantum nanowire is able to accommodate Majorana modes, [4]. The Hamiltonian of the lattice model corresponds to an $1D$ tight-binding lattice of spinless fermions, which under second quantization's language reads as

$$H = -\mu \sum_{i=1}^{N_s} n_i - \sum_{i=1}^{N_s-1} \left[t \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right) - \Delta \left(c_i c_{i+1} + c_{i+1}^\dagger c_i^\dagger \right) \right], \tag{2.1}$$

where $c_i^\dagger / c_i$ is a fermionic operator creating/annihilating an electron at site " i " and $n_i = c_i^\dagger c_i$ is the corresponding occupation number operator, μ is the chemical potential, $t \geqslant 0$ the hopping amplitude and $\Delta \geqslant 0$ the p-wave pairing amplitude[1]. Obviously N_s in the number of sites available within the limits of the lattice, setting the upper bound for the number electrons to $N \leqslant N_s$.

The first term is interpreted as a constant shift of the energy over all fermions, while their hopping from site i to a neighbouring site $i \pm 1$ is allowed for the price of a quantum of energy t, according to the second term. The last term - responsible for the p-wave pairing - shows the superconducting amplitude for the creation/annihilation of Cooper pairs from neighbouring fermions.

2.1 The "Intermezzo" of quantization schemes

A system introduced in second quantization's language, like the above-mentioned, does miss the underlying information of the single-particle Hamiltonian, which shows the fundamental degrees of freedom defined by the physical processes at microscopic level. The performance stage for a second quantized Hamiltonian, like the one of eq.(2.1), is the Fock space built from the blocks of the single-particle Hibert space. But, let me be a bit more precise and scientific about it...

[1] Note that the original Hamiltonian given by Kitaev [4] considers $\Delta \in \mathbb{C}$, introducing a superconducting phase ϕ in the Hamiltonian such that it reads $H = -\mu \sum_{i=1}^{N_s} n_i - \sum_{i=1}^{N_s-1} \left(t c_i^\dagger c_{i+1} - |\Delta| e^{i\phi} c_i c_{i+1} + h.c. \right)$. Having set $\phi = 0$ corresponds to performing a unitary transformation on H such that no generality is lost.

2.1.1 Introduction to Fock space

"Once upon a time, there was a spinless particle of mass "m" living in an 1D world coordinated by "x" and dictated by its Hamiltonian "H". The particle was always accompanied by its fellow wave-function $\psi(x,t) = \psi(x)e^{-\frac{i}{\hbar}Et}$ that belonged to a Hilbert space of functions, usually named as $\mathcal{H}^1$..."

Erwin Schrödinger taught us that a system like the above-mentioned satisfies his homonymous time-independent equation

$$H\psi(x) = \left(-\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial x}\right)^2 + V_{ex}(x)\right)\psi(x) = E\psi(x), \tag{2.2}$$

where $\hbar$ is the reduced Planck's constant, namely called Dirac's constant and $V_{ex}(x)$ is a potential imposed by the particle's environment. Once the explicit form of the potential $V_{ex}(x)$ allows analytical solutions to eq.(2.2), we discover a set of energy eigenvalues E_n and eigenstates or eigenfunctions $\psi_n(x)$ which form an orthogonal and complete basis for $\mathcal{H}^1$.

Introducing more than one non-interacting particle in the $1D$ world proposed, suggests the grand-canonical Hamiltonian of an $1D$ system of N identical particles, namely

$$H_{1D} = \sum_{i=1}^{N}\left(-\frac{\hbar^2\nabla^2}{2m} - \mu + V_{ex}(x_i)\right), \tag{2.3}$$

where x_i is the position of the i-th particle out of the N particles and μ is the chemical potential. Inevitably, the many-particle Schrödinger equation corresponding to our system is

$$i\hbar\frac{\partial}{\partial t}\Psi(x_1,...,x_N,t) = \sum_{i=1}^{N}\left(-\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial x_i}\right)^2 - \mu + V_{ex}(x_i)\right)\Psi(x_1,...,x_N,t), \tag{2.4}$$

where $\Psi(x_1,...,x_N,t)$ is the wave-function of the N-particle system belonging in the tensor product space $\mathcal{H}^N = \bigotimes_{n=1}^{N}\mathcal{H}^1 = \underbrace{\mathcal{H}^1\otimes\mathcal{H}^1\otimes\ldots\otimes\mathcal{H}^1}_{N\,\text{times}}$. Mathematically, it corresponds to a Slater determinant (fermions) or permanent (bosons) of a set of N single-particle wave-functions $\psi(x_i,t) = \psi(x_i)e^{-\frac{i}{\hbar}E_i t}$ that belong to the single-particle Hilbert space $\mathcal{H}^1$.

In the last paragraph we characterised the Hamiltonian given by eq.(2.3) as grand-canonical since a chemical potential term was introduced, although eq.(2.4) does require the number of particles to be specified, such that the dimensionality of the Hilbert space $\mathcal{H}^N$ is set and a solution $\Psi(x_1,...,x_N,t)$ can be found. Recalling that the grand-canonical scheme requires the number of particles to be unspecified, we need to amount on Fock space; this is the direct sum of tensor product copies of the single-particle Hilbert space $\mathcal{H}^1$, mathematically represented as

$$\mathcal{F} = \bigoplus_{N=0}^{+\infty}\mathcal{H}^N = \mathcal{H}^0\oplus\mathcal{H}^1\oplus\underbrace{\left(\mathcal{H}^1\otimes\mathcal{H}^1\right)}_{\mathcal{H}^2}\oplus\ldots\oplus\underbrace{\left(\mathcal{H}^1\otimes\mathcal{H}^1\otimes\ldots\otimes\mathcal{H}^1\right)}_{\mathcal{H}^N}\oplus\ldots, \tag{2.5}$$

where $\mathcal{H}^0 = \mathbb{C}|0\rangle$ representing the vacuum.

Working in the grand-canonical ensemble requires the introduction of creation/annihilation field operators $c^\dagger(x)/c(x)$ that act in $\mathcal{F}$ and satisfy the (anti-)commutation relations of the Clifford algebra respective to the nature of the system. This is defined by the following fermionic

anti-commutation relations

$$\{c(x), c(x')\} = \{c^\dagger(x), c^\dagger(x')\} = 0 \quad \& \quad \{c(x), c^\dagger(x')\} = \delta(x-x') \tag{2.6}$$

or bosonic commutation relations

$$[c(x), c(x')] = [c^\dagger(x), c^\dagger(x')] = 0 \quad \& \quad [c(x), c^\dagger(x')] = \delta(x-x'). \tag{2.7}$$

Their operation is physically interpreted as the addition/substraction of particles the ensemble. Subsequently, an arbitrary state of N particles $|\Psi(t)\rangle_N \in \mathcal{H}^N$ takes the form

$$|\Psi(t)\rangle_N = \frac{1}{\sqrt{N!}} \left(\prod_{i=1}^{N} \int dx_i \right) \Psi(x_1,...,x_N,t)\, c^\dagger(x_1) c^\dagger(x_2) \dots c^\dagger(x_N)|0\rangle\,, \tag{2.8}$$

if particles are labeled by subscript i, while the Hamiltonian dresses up in its second quantization's garment

$$H = \int dx\, c^\dagger(x) \left(-\frac{\hbar^2}{2m} \left(\frac{\partial}{\partial x_i} \right)^2 - \mu + V_{ex}(x) \right) c(x)\,, \tag{2.9}$$

satisfying the second quantized Schrödinger's equation $H|\Psi(t)\rangle_N = -i\hbar\partial_t|\Psi(t)\rangle_N$[2] if eq.(2.4) is satisfied.

2.1.2 The tight-binding model

Proceeding, allow us to pose restrictions on the previous system introduced by the second quantized Hamiltonian for non-interacting particles, eq.(2.9) to discover a well-known structure of solid state physics. The story continues as...

"One day, the spinless particle's 1D world was populated by more of his own kind, named as "fermions" while a periodic potential $V_{ex}(x_i) = V_{ex}(x_i + l\alpha)$, $l \in \mathbb{Z}$ & $\alpha \in \mathbb{R}$ rose as the ruler, bringing order."

Clearly, the creation/annihilation operators obey the anti-commutation relations of eq.(2.6) while the periodic potential $V_{ex}(x_i) = V_{ex}(x_i + l\alpha)$ makes an $1D$ lattice structure form, with α being the lattice site spacing of N_s sites able to host N fermions as $N_s \geqslant N$.

According to Bloch's Theorem, the periodicity of our system requires a specific type of solution for the single-particle wave-function $\psi(x)$. The wave-function describes a fermion delocalised across the lattice which satisfies eq.(2.2) while it has the form

$$\psi(x) = \psi_{n,k}(x) = e^{\mathbf{i}kx} u_{n,k}(x)\,, \tag{2.10}$$

where the function $u_{n,k}(x)$ is periodic. Its periodicity is in accordance to the lattice structure, such that $u_{n,k}(x) = u_{n,k}(x + l\alpha)$. The index n refers to the n-th energy band and k is the wavenumber of the fermion's momentum. A complementary single-particle basis of states is the complete and orthonormal set of Wannier functions $w_n(x-\alpha_i)$ which describe a fermion being localised around lattice points α_i with its wave-function being expressed as

$$\psi_{n,k}(x) = \frac{1}{\sqrt{N_s}} \sum_{i=1}^{N_s} e^{\mathbf{i}k\alpha_i} w_n(x-\alpha_i)\,, \tag{2.11}$$

[2] In case the reader would like to establish the equivalence between first and second quantization in detail - regarding calculations - please refer to textbooks such as [5],[6],[7],[8],[9].

where n is the same band index of the Bloch states and i is the site index.

At this point, let me introduce operators $c^\dagger_{n,i}/c_{n,i}$ that create/annihilate fermions in band n at a lattice site i in the Wannier state $w_n(x-\alpha_i)$. Expressing the fermionic field operators $c^\dagger(x)/c(x)$ in terms of the newly introduced $c^\dagger_{n,i}/c_{n,i}$

$$c^\dagger(x) = \sum_n w_n^*(x-\alpha_i)\, c^\dagger_{n,i} \quad \& \quad c(x) = \sum_n w_n(x-\alpha_i)\, c_{n,i}\,, \tag{2.12}$$

which, once inserted in the Hamiltonian of eq.(2.9), results in

$$H = \sum_{m,n} \left(-\mu \sum_{i=1}^{N_s} \delta_{mn} c^\dagger_{m,i} c_{n,i} - \sum_{i,j=1}^{N_s} t_{ij}^{mn} c^\dagger_{m,i} c_{n,j} \right), \tag{2.13}$$

where the hopping amplitude t_{ij}^{mn} among different sites i, j corresponds to

$$t_{ij}^{mn} = \int dx \left(w_m^*(x-\alpha_i) \left(-\frac{\hbar^2}{2m} \left(\frac{\partial}{\partial x} \right)^2 + V_{ex}(x) \right) w_n(x-\alpha_j) \right). \tag{2.14}$$

Those Wannier states form a reasonable choice within the tight-binding limit. According to the tight-binding approach, the lattice structure consists of tightly bound fermions around equilibrium points α_i which are assumed minima of the periodic potential $V_{ex}(x+l\alpha)$. Therefore, it allows us to approximate the potential around each fermion by a harmonic oscillator potential

$$V_{ex}(x) = \cancel{V_{ex}(\alpha_i)} + \cancel{V'_{ex}(\alpha_i)(x-\alpha_i)} + \frac{1}{2} V''_{ex}(\alpha_i)(x-\alpha_i)^2 + ... \tag{2.15}$$

for $(x-\alpha_i) \ll \alpha$; as $V_{ex}(\alpha_i) = const$, so it can be omitted and $V'_{ex}(\alpha_i) = 0$ as the minima of the potential are situated at $x = \alpha_i$.

Consequently, the Wannier states correspond to the well known harmonic oscillator wave-functions. Defining

$$m\omega^2 = V''_{ex}(\alpha_i) = \left. \frac{d^2 V_{ex}(x)}{dx^2} \right|_{x=\alpha_i}, \tag{2.16}$$

gives us

$$w_n(x-\alpha_i) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-\frac{m\omega(x-\alpha_i)^2}{2\hbar}} H_n\left(\sqrt{\frac{m\omega}{\hbar}} (x-\alpha_i) \right), \tag{2.17}$$

where $H_n(x)$ is the n-th Hermite polynomial given by the expression

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} \left(e^{-x^2} \right). \tag{2.18}$$

Therefore, the single-particle state corresponding to our tight-binding lattice of fermions is

$$\psi_{n,k}(x) = \frac{1}{\sqrt{N_s}} \sum_{i=1}^{N_s} e^{\mathbf{i}k\alpha_i} \frac{\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}}{\sqrt{2^n n!}} e^{-\frac{m\omega(x-\alpha_i)^2}{2\hbar}} H_n\left(\sqrt{\frac{m\omega}{\hbar}} (x-\alpha_i) \right), \tag{2.19}$$

which forms a complete basis on $\mathcal{H}^1$. Of course the many-particle wave-function $\Psi(x_1,...,x_N,t) \in \mathcal{H}^N$ is no other than the Slater determinant of the orthogonal and complete set of $\psi_{n,k}(x_i)$, where $i = 1,2,\ldots,N$.

Further more, since the tight-binding limit is considered, as long as the kinetic energy of fermions due to temperature T is significantly smaller that their potential term, specifically if $k_B T \ll \frac{\hbar}{m^2}\sqrt{\frac{d^2 V_{ex}(a_i)}{dx^2}}$, a single-band approximation is sufficient. Secondly, only nearest neighbour hopping is considered, simplifying eq.(2.13) to

$$H = -\mu \sum_{i=1}^{N_s} c_i^\dagger c_i - t \sum_{i=1}^{N_s} \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right), \tag{2.20}$$

which is obviously equal to eq.(2.1) for $\Delta = 0$.

2.1.3 The superconducting gap Δ

Establishing a connection with Kitaev's Hamiltonian, eq.(2.1), addresses a question about the microscopic processes disguised as Δ. So in the upcoming section I will sketch an explanation, trying to give an insight into it.

We start with the addition of a two-body interaction term among fermions to the many-particle Hamiltonian of eq.(2.3)

$$\frac{1}{2} \sum_{i,j=1}^{N} V(x_i - x_j), \tag{2.21}$$

where $i \neq j$, which subsequently leads to the addition of the following term in the second quantized version of the Hamiltonian given by eq.(2.9)

$$H_{int} = \frac{1}{2} \int dx \int dy\, c^\dagger(x) c^\dagger(y) V(x-y) c(x) c(y). \tag{2.22}$$

Approximating the interaction as a mean-field suggests that

$$H_{int} \propto \left\langle c^\dagger(x) V(x-y) c^\dagger(y) \right\rangle c(x) c(y) + c^\dagger(x) c^\dagger(y) \left\langle c(x) V(x-y) c(y) \right\rangle, \tag{2.23}$$

where the braces $\langle \dots \rangle$ denote averaging, or

$$H_{int} \approx \int dx \int dy \left(\Delta^\dagger(x,y)\, c(x) c(y) + \Delta(x,y)\, c^\dagger(x) c^\dagger(y) \right), \tag{2.24}$$

where obviously $\Delta(x,y) = \left\langle c(x) V(x-y) c(y) \right\rangle$. This is called the superconducting gap and it corresponds physically to a correlation function among different fermions, weighted by their interaction.

Finally, inserting eq.(2.12) in the single-band approximation and considering only nearest neighbour coupling, transforms the above-mentioned term to

$$H_{int} = \sum_{i=1}^{N_s - 1} \left(\Delta^* c_i c_{i+1} + \Delta\, c_{i+1}^\dagger c_i^\dagger \right). \tag{2.25}$$

2.2 Bulk properties & dispersion relations

In the the previous section we investigated the tight-binding lattice model building bridges between the first and second quantization schemes. Even though we showed the explicit form of single-particle eigenfunctions, we understand that the exact form of the Wannier states is

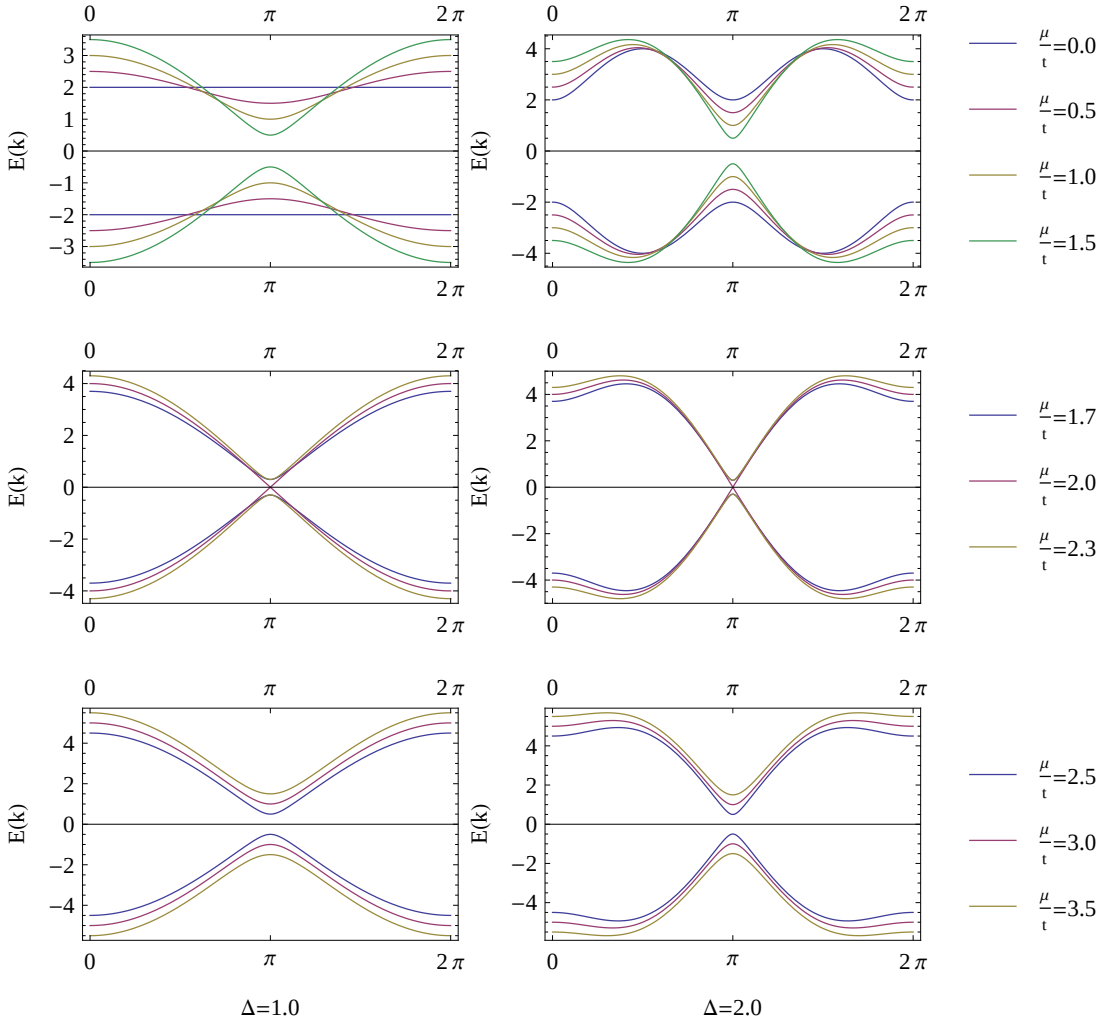

Figure 2.1: The dispersion relation of an $1D$ spinless p-wave superconductor. In the bottom row we encounter the trivially superconducting gapped phase, $|\mu| > 2t$ and in the first row the topological one, $|\mu| < 2t$. The middle row shows the transitional regime of $\mu = \pm 2t$. The first column corresponds to $\Delta = t$ while the second to $\Delta \neq t$.

indifferent to us; as long as they form a complete basis of states allowing us to write expansions for the field operators, like in eq.(2.12).

A useful property of the Wannier states is that they are orthogonal by definition and related to the Bloch states through a discrete Fourier transformation, eq.(2.11). The same transformation applied to the creation/annihilation operators gives us their representation in momentum k-space. Later on, it will allow us to uncover the dispersion relation for the system. So, the Fourier transformated expansion of the operators is

$$c_i^\dagger = \frac{1}{\sqrt{N_s}} \sum_k e^{-\mathbf{i}k\alpha i} c_k^\dagger, \quad c_i = \frac{1}{\sqrt{N_s}} \sum_k e^{\mathbf{i}k\alpha i} c_k, \tag{2.26}$$

where $0 \leq k \leq \frac{2\pi m}{\alpha N_s}$ and $m = 0, 1, .., N_s$. Applying eq.(2.26) to Kitaev's Hamiltonian (2.1) results in its Fourier transformed version

$$H = \sum_k \left(-\mu - 2t \left(1 - \frac{1}{N_s}\right) \cos(k\alpha) \right) c_k^\dagger c_k + \Delta \left(1 - \frac{1}{N_s}\right) \sum_k \left(e^{\mathbf{i}k\alpha} c_{-k} c_k + e^{-\mathbf{i}k\alpha} c_k^\dagger c_{-k}^\dagger \right), \tag{2.27}$$

of the Kitaev's lattice; for the explicit calculation please check Appendix B.

The term $(1 - 1/N_s)$ is a consequence of the open boundary condition imposed in Kitaev's model. Imposing a periodic boundary condition on the lattice - actually wrapping the lattice around its ends such that $N_s + 1 = 1$ - makes $(1 - 1/N_s) \to 1$ and is equivalent to the case of considering an lattice of infinite length, so letting $N_s \to +\infty$. In other words, uncovering the bulk properties of Kitaev's model is equivalent to writing the Hamiltonian as

$$H = \sum_k \varepsilon_k c_k^\dagger c_k + \Delta \sum_k \left(e^{\mathbf{i}k\alpha} c_{-k} c_k + e^{-\mathbf{i}k\alpha} c_k^\dagger c_{-k}^\dagger \right), \tag{2.28}$$

where $\varepsilon_k = -\mu - 2t\cos(k\alpha)$. Please note that ε_k is a dispersion relation of a non-superconductive ($\Delta = 0$) tight-binding lattice, dictating the well known electronic band structure of metals.

Proceeding, we employ the Bogoliubov - de Gennes form for the above-mentioned bulk Hamiltonian, eq.(2.28). Introducing the 2-component operator $(c_k^\dagger, c_{-k})$, makes us express it in the form

$$H = \frac{1}{2} \sum_k \begin{pmatrix} c_k^\dagger & c_{-k} \end{pmatrix} \begin{pmatrix} \varepsilon_k & \Delta_k \\ \Delta_k^* & -\varepsilon_k \end{pmatrix} \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix}, \tag{2.29}$$

where now $0 \leq k \leq 2\pi$ and $\Delta_k = -2i\Delta\sin(k\alpha)$. Consecutively, diagonalizing H brings it to the form

$$H = \sum_k E(k) \tilde{c}_k^\dagger \tilde{c}_k. \tag{2.30}$$

Here it is expressed in terms of the quasi-fermion operators

$$\tilde{c}_k = u_k c_k + \upsilon_k c_{-k}^\dagger, \tag{2.31}$$

where

$$u_k = \frac{\Delta_k}{|\Delta_k|} \sqrt{\frac{E(k) + \varepsilon_k}{2E(k)}} \quad \text{and} \quad \upsilon_k = \frac{E(k) - \varepsilon_k}{\Delta_k}. \tag{2.32}$$

The diagonalized form of eq.2.30 delivers an intuitively transparent dispersion relation $E(k)$ for the positive/negative energy modes of the bulk spectrum, namely

$$E(k) = \pm\sqrt{\varepsilon_k^2 + |\Delta_k|^2} = \pm\sqrt{(\mu + 2t\cos(k\alpha))^2 + (2\Delta\sin(k\alpha))^2}. \tag{2.33}$$

Once the dispersion relation is plotted, see fig.2.1, it shows that the spectrum is gapped unless the chemical potential is tuned at $\mu = \pm 2t$.

According to J. Alicea's review paper [10], the two gapped phases of $|\mu| > 2t$ and $|\mu| < 2t$ correspond to different Couper-pairing regimes. If we examine the quasi-fermions ground state $|g.s.\rangle$, which satisfies the defining relation $\tilde{c}_k |g.s.\rangle = 0$, we find out that

$$|g.s.\rangle \propto \prod_{0<k<\pi} \left(1 + \phi_{c.p.}(k) c_{-k}^\dagger c_k^\dagger\right) |0\rangle, \tag{2.34}$$

with $|0\rangle$ being the vacuum for fermions created by $c_k^\dagger$ and $\phi_{c.p.}(k) = \upsilon_k / u_k$. The former ratio, $\phi_{c.p.}(k)$, can be interpreted as the wave-function of a Cooper pair formed by two fermions with opposite momentum k. It's Fourier transform, $\phi_{c.p.}(x)$, in the real space shows that for large x

$$\phi_{c.p.}(x) = \int \phi_{c.p.}(x) e^{ikx}\, dk \overset{x\gg 0}{\Longrightarrow} |\phi_{c.p.}(x)| \sim e^{-|x|/\zeta}, \quad \zeta \in \mathbb{R}. \tag{2.35}$$

It has been shown by N. Read and D. Green in [11] that if $|\mu| > 2t$ "*two fermions bound in real space over a length scale* ζ" refering to a strong-pairing coupling while in the weak-pairing regime, $|\mu| < 2t$, the length scale becomes infinite, $\zeta \to \infty$ and $\phi_{c.p.}(x) \sim const$. The strong versus the weak-pairing regimes are characterised as trivial and topological respectively. In fig.2.1 we plot the dispersion relation for the trivial and the topological regimes, which are gapped, but also the gapless spectrum at the boundary $\mu = \pm 2t$.

2.3 Split the fermions, Majoranas rise!

At this point, after having a well-defined system under the Kitaev Hamiltonian being investigated about it's bulk spectrum properties, it's time to start performing the magic spells of Majorana. Already in section 1.3 we proposed that a fermion can be "split" into its real and imaginary part; applying such an suggestion in Kitaev's Hamilitonian, eq.(2.1), means

$$\begin{aligned} H &= -\mu \sum_{i=1}^{N_s} n_i - \sum_{i=1}^{N_s-1} \left[t \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right) - \Delta \left(c_i c_{i+1} + c_{i+1}^\dagger c_i^\dagger \right) \right] \\ &\Updownarrow eq.(1.8) \\ H &= -\mu \sum_{i=1}^{N_s} \frac{1}{2} \left(1 + i\gamma_{2i-1}\gamma_{2i} \right) - \frac{i}{2} \sum_{i=1}^{N_s-1} \left[(t-\Delta)\gamma_{2i-1}\gamma_{2i+2} - (t+\Delta)\gamma_{2i}\gamma_{2i+1} \right], \end{aligned} \tag{2.36}$$

where we can see how μ, t and Δ couple the Majorana operators.

In order to understand the physics of the system transparently, we suggest treating Kitaev's Hamiltonian, eq.(2.36), for two simplified cases which will show how that coupling induced among the Majoranas results in different phases. Kitaev suggests in [4] that the strong $(\mu > 2t)$ and weak-pairing regimes $(\mu < 2t)$ corresponding to the trivial and the topological phases respectively, are conjectured with those two simpified cases. Namely, the cases for the coupling between the Majoranas are:

$(a)\, \mu \neq 0\,,\, t = \Delta = 0$: The Hamiltonian $H = -\mu \sum_{i=1}^{N_s} \frac{1}{2} \left(1 + i\gamma_{2i-1}\gamma_{2i} \right) = -\mu \sum_{i=1}^{N_s} n_i$ shows that Majoranas from the same i-th site couple forming fermions of a trivial $1D$ lattice structure, where the addition or subtraction of an ordinary fermion involves an energy exchange of μ.

$(b)\, \mu = 0\,,\, t = \Delta \neq 0$: In this special case only the last term of the above-mentioned eq.(2.36) will survive, such that the Hamiltonian

$$H = it \sum_{i=1}^{N_s-1} \gamma_{2i}\gamma_{2i+1} \tag{2.37}$$

shows how the Majorana operators combine in a non-trivial way; specifically between neighbouring sites i and $i+1$ as you can also observe in the lower part of fig.2.3.

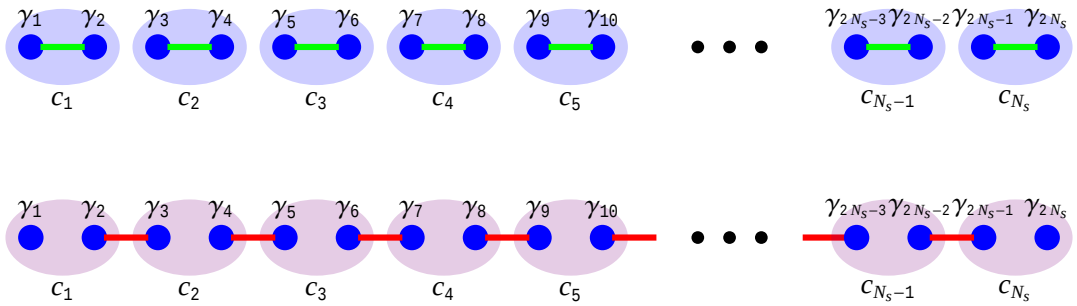

Figure 2.2: The couplings of Majorana operators in Kitaev's lattice model. The upper lattice corresponds to the trivial coupling of case (a) conjectured with the strong-pairing regime. The bottom line corresponds to the non-trivial case of (b) conjectured with the weak-pairing regime which shows a topological phase.

As case (a) suggests, using a non-zero chemical potential, $\mu \neq 0$, is equivalent to a constant shift of the energy spectrum by μ. So, setting $\mu = 0$ in case (b) was only for the sake of clarity on the demonstration of the non-trivial coupling. Keeping our attention focused on that, let me try a mathematical trick on the Hamiltonian given by eq.(2.37) and by the end, I will show a little piece of jewellery that is on the table and asking for attention. So if

$$H = it \sum_{i=1}^{N_s-1} \gamma_{2i}\gamma_{2i+1} = t \sum_{i=1}^{N_s-1} \frac{1}{2}\left(1 + 2i\gamma_{2i}\gamma_{2i+1} + 1 - 2\right) \tag{2.38}$$

according to the Clifford algebra suggested in section 1.3 I am allowed to consider ${\gamma_i}^2 = 1$ and claim that

$$H = t \sum_{i=1}^{N_s-1} \frac{1}{2}\left(\gamma_{2i}\gamma_{2i} - i\gamma_{2i+1}\gamma_{2i} + i\gamma_{2i}\gamma_{2i+1} + \gamma_{2(i+1),1}\gamma_{2(i+1)} - 2\right). \tag{2.39}$$

Rewriting the above expression as

$$H = 2t \sum_{i=1}^{N_s-1} \left[\left(\frac{\gamma_{2i} + i\gamma_{2i+1}}{2}\right)^{\dagger}\left(\frac{\gamma_{2i} + i\gamma_{2i+1}}{2}\right) - \frac{1}{2}\right], \tag{2.40}$$

suggests the following combinations of Majorana operators

$$\tilde{c}_i = \frac{1}{2}(\gamma_{2i} + i\gamma_{2i+1}), \qquad \tilde{c}_i^{\dagger} = \frac{1}{2}(\gamma_{2i} - i\gamma_{2i+1}), \tag{2.41}$$

which are fermionic, while the Hamiltonian becomes

$$H = 2t \sum_{i=1}^{N_s-1} \left(\tilde{n}_i - \frac{1}{2}\right), \tag{2.42}$$

proposing a trivial $1D$ lattice structure! The addition or subtraction of a quasi-fermion involves an energy exchange of $2t$, since $\tilde{n}_i = \tilde{c}_i^{\dagger}\tilde{c}_i$ while the ground state is at $E = -t$. Let me say that I managed to "majoranate" the original Hamiltonian in eq.(2.37) and "refermioned" it in eq.(2.42). But since case (b) is conjectured with the topological phase of the bulk lattice, as explained

in section 2.2, our qualitative conclusions hold if the chemical potential lies within the weak-pairing regime, $|\mu| < 2t$. This motivates us to focus on the case of $\mu = 0$ for the rest of this chapter and discard case (a).

Alright, so far all is mathematically coherent and nicely reformulated, so it's time to pose meaningful questions. Where are the Majorana's? Is the form of the the Hamiltonian in eq.(2.37) revealing them? It only looks as the result of an intermediate step of a mathematical trick through which we diagonalized the original Hamiltonian, eq.(2.1) and "along the way" the operators introduced by eq.(1.4), happened to qualify for Majorana fermion's creation/ annihilation operators! But... a rigorous look at the diagonalized Hamiltonian of eq.(2.37), shows that the Majorana operators γ_1 and γ_{N_s} are missing! These are the Majorana fermions that we are seeking, as these non neighbouring site operators - both are localised at the ends of our lattice - do give rise to physically realisable Majorana fermions. The emerging Majoranas can be expressed as the non-local quasi-fermionic state

$$\tilde{c}_M^\dagger = \frac{\gamma_{N_s} - i\gamma_1}{2} \tag{2.43}$$

of zero-energy cost, since they are not included in the Hamiltonian! Then, equipping ourselves with a ground state $|0\rangle$ that satisfies the condition $\tilde{c}_M|0\rangle = 0$ will inevitably give us a counterpart ground state $|1\rangle = \tilde{c}_M^\dagger|0\rangle$ that doubles the degeneracy and makes non-Abelian statistics rise! The zero-energy cost at which this ground state non-local fermion exists makes it the ideal candidate for a qubit!

2.4 Uncovering the ground state

In the last two sections, the Hamiltonian of the Kitaev model (2.1) has been manipulated by transformations in such a way that we uncovered a dispersion relation in 2.2 and diagonalized it for the case of $\mu = 0, t = \Delta$ in section 2.3, by introducing quasi-fermions $\tilde{c}_i$. By the end of section 2.3 it was discovered that there is a quasifermionic non-local state created by $\tilde{c}_M^\dagger$ at zero-energy. The question that naturally rises is whether a ground state exists on which the state $\tilde{c}_M$ or $\tilde{c}_M^\dagger$ is superposed at the expense of no energy. May our dream for a degenerate state at $E = 0$ come true; then non-Abelian statistics rise, as we wished for since the introduction. Trying to shed light on the above-mentioned questions, on this section we seek for the eigenstates of the Kitaev model in the occupation number representation.

2.4.1 The 2-site lattice for $\mu = 0$, $t = \Delta$

Starting easy, we are going to treat a 2-site lattice for the special case of $\mu = 0, t = \Delta$ of Kitaev's Hamiltonian which reads as

$$H = -t(c_1^\dagger c_2 + c_2^\dagger c_1 - c_1 c_2 - c_2^\dagger c_1^\dagger). \tag{2.44}$$

Accompanied by the vacuum state $|00\rangle$ - representing the total absence of electrons - makes us easily form the set of states

$$|00\rangle, |10\rangle = c_1^\dagger|00\rangle, |01\rangle = c_2^\dagger|00\rangle \quad \& \quad |11\rangle = c_1^\dagger c_2^\dagger|00\rangle \tag{2.45}$$

and calculate its occupation number representation matrix form

$$H = \begin{pmatrix} \langle 00|H|00\rangle & \langle 00|H|10\rangle & \langle 00|H|01\rangle & \langle 00|H|11\rangle \\ \langle 10|H|00\rangle & \langle 10|H|10\rangle & \langle 10|H|01\rangle & \langle 10|H|11\rangle \\ \langle 01|H|00\rangle & \langle 01|H|10\rangle & \langle 01|H|01\rangle & \langle 01|H|11\rangle \\ \langle 11|H|00\rangle & \langle 11|H|10\rangle & \langle 11|H|01\rangle & \langle 11|H|11\rangle \end{pmatrix}, \tag{2.46}$$

namely being

$$H = \begin{pmatrix} 0 & 0 & 0 & -t \\ 0 & 0 & -t & 0 \\ 0 & -t & 0 & 0 \\ -t & 0 & 0 & 0 \end{pmatrix}. \tag{2.47}$$

Subsequently, diagonalizing the matrix form of the Hamiltonian above, shows that

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} -t & 0 & 0 & 0 \\ 0 & -t & 0 & 0 \\ 0 & 0 & t & 0 \\ 0 & 0 & 0 & t \end{pmatrix} \cdot \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ -1 & 0 & 0 & 1 \\ 0 & -1 & 1 & 0 \end{pmatrix}, \tag{2.48}$$

uncovering a doubly degenerate spectrum of two energy eigenvalues, namely $E = \mp t$. The corresponding eigenvectors are the following

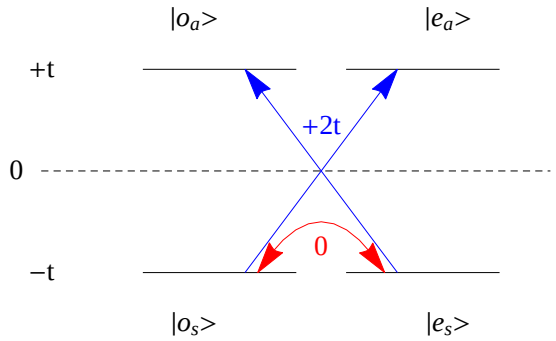

Figure 2.3: The 2-site lattice spectrum and it's excitations in occupation number base, $\Delta = t$.

$$|e_a\rangle = \frac{1}{\sqrt{2}}(-|00\rangle + |11\rangle), \quad E = +t, \tag{2.49}$$

$$|o_a\rangle = \frac{1}{\sqrt{2}}(-|10\rangle + |01\rangle), \quad E = +t, \tag{2.50}$$

$$|e_s\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle), \quad E = -t, \tag{2.51}$$

$$|o_s\rangle = \frac{1}{\sqrt{2}}(|10\rangle + |01\rangle), \quad E = -t, \tag{2.52}$$

which are also graphically depicted in fig.(2.4.1). The blue lines represent the allowed excitations from the two-fold degenerate ground state $|e/o_s\rangle$, while the red one represents the interchange between the ground states. Please, note that the excitation $|e/o_s\rangle \leftrightarrow |e/o_a\rangle$ is not depicted. The reason is that when we calculate the spectrum using the Nambu base, section 2.4.2, it will be found that it is not allowed.

Clearly the ground state consists of the symmetric states $|e_s\rangle$ and $|o_s\rangle$ - so it is doubly degenerate - with even/odd parity making the distinction. Parity corresponds to the even/odd number of fermions in the states and is measured by the operator $P = \prod_{i=1}^{N_s} (-i\gamma_{2i-1}\gamma_{2i})$, as suggested by Kitaev [4]. In our 2-site lattice case, it reads $P = -i\gamma_1\gamma_4$. Then since

$$P|e_s\rangle = -i\gamma_1\gamma_4|e_s\rangle = (+1)|e_s\rangle \quad \& \quad P|o_s\rangle = -i\gamma_1\gamma_4|o_s\rangle = (-1)|o_s\rangle, \tag{2.53}$$

the name even/odd parity state for $|e_s\rangle/|o_s\rangle$ respectively, is justified.

Now, further treatment of the occupation number eigenstates is needed, such that those states are connected to the states of the "refermioned" diagonal Hamiltonian of eq.(2.42). Rewriting the occupation number operator for the quasi-fermions $\tilde{n}_1$ in terms of fermions

$$\tilde{n}_1 = \tilde{c}_1^\dagger \tilde{c}_1 = \frac{1}{2}(1 + i\gamma_2\gamma_3) = \frac{1}{2}(1 - c_1^\dagger c_2 - c_2^\dagger c_1 - c_2 c_1 - c_1^\dagger c_2^\dagger) \tag{2.54}$$

and acting on the eigenstates gives us

$$\tilde{n}_1|e_s\rangle = \tilde{n}_1|o_s\rangle = 0, \quad \text{while} \quad \tilde{n}_1|e_a\rangle = |e_a\rangle \quad \& \quad \tilde{n}_1|o_a\rangle = |o_a\rangle. \tag{2.55}$$

This shows that the symmetric ground states $|e_s\rangle$, $|o_s\rangle$ correspond to the vacuum of quasi-fermions while the anti-symmetric excited states $|e_a\rangle, |o_a\rangle$ to the occupied states. Of course acting with $\tilde{c}_1^\dagger$ on the quasi-fermion vacuum states, the symmetric states $|e/o_s\rangle$, results in the occupied antisymmetric states $|o/e_a\rangle$ respectively, as

$$\tilde{c}_1^\dagger|e_s\rangle = |o_a\rangle \quad \& \quad \tilde{c}_1^\dagger|o_s\rangle = |e_a\rangle. \tag{2.56}$$

In other words, the operator $\tilde{c}_1^\dagger$ makes the quasi-fermion vacuum states populate and exchange parity.

Secondly, using the table 2.1, we calculate the effect of the non-local zero-energy quasi-fermionic creation/annihilation operator $\tilde{c}_M^\dagger / \tilde{c}_M$ on the energy eigenstates. We discover that

$$\begin{aligned} \tilde{c}_M^\dagger|e_s\rangle = 0, \qquad & \tilde{c}_M|e_s\rangle = +i|o_s\rangle, \\ \tilde{c}_M|o_s\rangle = 0, \qquad & \tilde{c}_M^\dagger|o_s\rangle = -i|e_s\rangle \end{aligned}$$

and subsequently $\tilde{c}_M^\dagger \tilde{c}_M|e_s\rangle = |e_s\rangle$. Therefore we should consider the odd ground state $|o_s\rangle = |0\rangle$, where $|0\rangle$ is the qubit candidate state discussed by the end of section 2.3. Subsequently, the counterpart state is recognised as $|1\rangle = -i|e_s\rangle$.

As a final part, let us investigate how the action of γ_i operators affects the energy eigenstates, making them switch from one to another. Considering all possible combinations $\gamma_i|e/o_{a/s}\rangle$ we create table 2.1 shown on the right.

	$\lvert e_s\rangle$	$\lvert o_s\rangle$	$\lvert e_a\rangle$	$\lvert o_a\rangle$
γ_1	$\lvert o_s\rangle$	$\lvert e_s\rangle$	$\lvert o_a\rangle$	$\lvert e_a\rangle$
γ_2	$+i\lvert o_s\rangle$	$-i\lvert e_s\rangle$	$-i\lvert o_a\rangle$	$+i\lvert e_a\rangle$
γ_3	$-\lvert o_a\rangle$	$-\lvert e_a\rangle$	$-\lvert o_s\rangle$	$-\lvert e_s\rangle$
γ_4	$+i\lvert o_s\rangle$	$-i\lvert e_s\rangle$	$-i\lvert o_a\rangle$	$+i\lvert e_a\rangle$

Table 2.1: Interchanges of energy states with majorana operators γ_i acting on the states.

2.4.2 The general case of a 2-site lattice for $\mu = 0$, $t \neq \Delta$

Dealing again with a 2-site lattice, but for the general case of $\mu = 0, t \neq \Delta \geqslant 0$ the Hamiltonian takes the explicit form

$$H = -t(c_1^\dagger c_2 + c_2^\dagger c_1) + \Delta(c_1 c_2 + c_2^\dagger c_1^\dagger), \tag{2.57}$$

accompanied by the usual occupation number representation eigenstates $|00\rangle, |10\rangle, |01\rangle$ and $|11\rangle$. Having those at hand as a basis, we calculate the matrix form of the Hamiltonian as before, resulting in

$$H = \begin{pmatrix} 0 & 0 & 0 & -\Delta \\ 0 & 0 & -t & 0 \\ 0 & -t & 0 & 0 \\ -\Delta & 0 & 0 & 0 \end{pmatrix} \tag{2.58}$$

and continue diagonalizing, such that

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 0 & 1 & -1 \\ 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{pmatrix} \cdot \begin{pmatrix} -t & 0 & 0 & 0 \\ 0 & t & 0 & 0 \\ 0 & 0 & -\Delta & 0 \\ 0 & 0 & 0 & \Delta \end{pmatrix} \cdot \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 1 & 0 \\ 0 & -1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ -1 & 0 & 0 & 1 \end{pmatrix}, \tag{2.59}$$

uncovering us the spectrum of eigenvalues $E = \mp t$ and $E = \mp\Delta$ and their corresponding eigenvectors

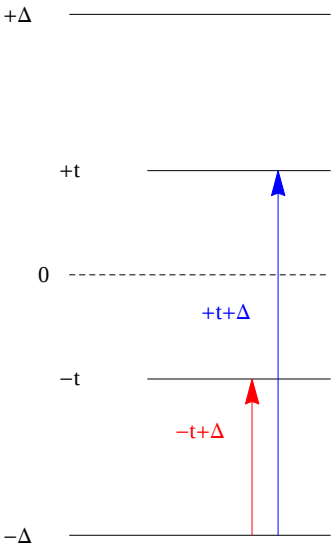

Figure 2.4: The 2-site lattice spectrum and it's excitations in occupation number base, $\Delta \neq t$.

$$|e_a\rangle = \frac{1}{\sqrt{2}}\left(-|00\rangle + |11\rangle\right), \quad E = +\Delta, \tag{2.60}$$

$$|o_a\rangle = \frac{1}{\sqrt{2}}\left(-|10\rangle + |01\rangle\right), \quad E = +t \tag{2.61}$$

$$|e_s\rangle = \frac{1}{\sqrt{2}}\left(|00\rangle + |11\rangle\right), \quad E = -\Delta, \tag{2.62}$$

$$|o_s\rangle = \frac{1}{\sqrt{2}}\left(|10\rangle + |01\rangle\right), \quad E = -t. \tag{2.63}$$

We can clearly see how setting $\Delta = t$ will give us all the results of the previous section 2.4.1. Please, note that now the degeneracy of the ground state $|e/o_s\rangle$ has been lifted since the energy levels of $\pm\Delta$ are separated from those for $\pm t$. This is clearly depicted on fig.2.4.2 where now the red and blue arrows depict the excitations from the ground state $|e_s\rangle$.

The Nambu base as an alternative one.

An alternative way of diagonalizing the 2-site lattice Hamiltonian, eq.(2.57), is by introducing the Nambu base $\Psi = (c_1, c_2, c_1^\dagger, c_2^\dagger)^\intercal$. Then eq.(2.57) can be written as

$$H = \frac{1}{2}\Psi^\dagger H_n \Psi, \tag{2.64}$$

with

$$H_n = \begin{pmatrix} 0 & -t & 0 & \Delta \\ -t & 0 & -\Delta & 0 \\ 0 & -\Delta & 0 & +t \\ \Delta & 0 & +t & 0 \end{pmatrix}. \tag{2.65}$$

Consecutively, diagonalizing it uncovers the eigenvalues $E = \pm(t \pm \Delta)$ and eigenvectors

$$\psi_1 = \frac{-1}{2}(1,1,1,-1)^\intercal, \quad E = -t - \Delta, \tag{2.66}$$

$$\psi_2 = \frac{1}{2}(1,1,-1,1)^\intercal, \quad E = -t + \Delta, \tag{2.67}$$

$$\psi_3 = \frac{1}{2}(-1,1,1,1)^\intercal, \quad E = t - \Delta, \tag{2.68}$$

$$\psi_4 = \frac{1}{2}(1,-1,1,1)^\intercal, \quad E = t + \Delta, \tag{2.69}$$

respectively. In the case of tuning $\Delta = t$ the eigenvalues spectrum shows a degeneracy at $E = 0$ while the eigenstates ψ_1 and ψ_4 seem to be separated in energy scale by $4t$. If we diagonalize eq.(2.65) once again, we discover that the eigenstates ψ_2 and ψ_3 have changed while ψ_1 and ψ_4 are the same. Namely, the spectrum is

$$\psi_1 = \frac{-1}{2}(1,1,1,-1)^\intercal, \quad E = -2t, \tag{2.70}$$

$$\psi_2 = \frac{1}{\sqrt{2}}(0,1,0,1)^\intercal, \quad E = 0, \tag{2.71}$$

$$\psi_3 = \frac{1}{\sqrt{2}}(-1,0,1,0)^\intercal, \quad E = 0, \tag{2.72}$$

$$\psi_4 = \frac{1}{2}(1,-1,1,1)^\intercal, \quad E = +2t, \tag{2.73}$$

showing that the degeneracy at $E = 0$ allows for a change in the form of the states ψ_2 and ψ_3 in the Nambu base.

2.4.3 The 3-site lattice

As a second step, I follow the same procedure for a 3-site lattice again for the special case of $\mu = 0, t = \Delta$ where the Hamiltonian is

$$H = -t(c_1^\dagger c_2 + c_2^\dagger c_1 - c_1 c_2 - c_2^\dagger c_1^\dagger + c_2^\dagger c_3 + c_3^\dagger c_2 - c_2 c_3 - c_3^\dagger c_2^\dagger) \tag{2.74}$$

and the accompanying occupation number representation eigenstates are

$$\begin{aligned}
&|000\rangle = \textit{Vacuum} \qquad (c_i|000\rangle = 0)\,,\\
&|100\rangle = c_1^\dagger|000\rangle, \quad |010\rangle = c_2^\dagger|000\rangle, \quad |001\rangle = c_3^\dagger|000\rangle,\\
&|110\rangle = c_1^\dagger c_2^\dagger|000\rangle, \quad |101\rangle = c_1^\dagger c_3^\dagger|000\rangle, \quad |011\rangle = c_2^\dagger c_3^\dagger|000\rangle,\\
&|111\rangle = c_1^\dagger c_2^\dagger c_3^\dagger|000\rangle.
\end{aligned}$$

The Hamiltonian's matrix representation follows, as

$$H = \begin{pmatrix}
0 & 0 & 0 & 0 & -t & 0 & -t & 0\\
0 & 0 & -t & 0 & 0 & 0 & 0 & -t\\
0 & -t & 0 & -t & 0 & 0 & 0 & 0\\
0 & 0 & -t & 0 & 0 & 0 & 0 & -t\\
-t & 0 & 0 & 0 & 0 & -t & 0 & 0\\
0 & 0 & 0 & 0 & -t & 0 & -t & 0\\
-t & 0 & 0 & 0 & 0 & -t & 0 & 0\\
0 & -t & 0 & -t & 0 & 0 & 0 & 0
\end{pmatrix}, \tag{2.75}$$

which we diagonalize. The results is the diagonalized Hamiltonian

$$\tilde{H} = \begin{pmatrix} -2t & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -2t & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2t & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2t & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \tag{2.76}$$

which uncovers the eigenvalue spectrum $\mp 2t, 0$ and the corresponding eigenvectors

$$\begin{aligned} |o_s\rangle &= \tfrac{1}{\sqrt{4}}\left(|100\rangle + |010\rangle + |001\rangle + |111\rangle\right), \qquad E = -2t \\ |e_s\rangle &= \tfrac{1}{\sqrt{4}}\left(|000\rangle + |110\rangle + |101\rangle + |011\rangle\right), \end{aligned}$$

$$\begin{aligned} |o_a\rangle &= \tfrac{1}{\sqrt{4}}\left(-|100\rangle + |010\rangle - |001\rangle + |111\rangle\right), \qquad E = +2t \\ |e_a\rangle &= \tfrac{1}{\sqrt{4}}\left(-|000\rangle + |110\rangle - |101\rangle + |011\rangle\right), \end{aligned}$$

$$\begin{aligned} |o_1\rangle &= \tfrac{1}{\sqrt{2}}\left(-|010\rangle + |111\rangle\right), \quad |e_2\rangle = \tfrac{1}{\sqrt{2}}\left(-|110\rangle + |011\rangle\right), \qquad E = 0 \\ |e_3\rangle &= \tfrac{1}{\sqrt{2}}\left(-|000\rangle + |101\rangle\right), \quad |o_4\rangle = \tfrac{1}{\sqrt{2}}\left(-|100\rangle + |001\rangle\right). \end{aligned}$$

For the the 3-site lattice case, the occupation number operator is

$$\tilde{n} = \tilde{c}_1^\dagger \tilde{c}_1 + \tilde{c}_2^\dagger \tilde{c}_2 = \frac{1}{2}(2 - c_1^\dagger c_2 - c_2^\dagger c_1 - c_2 c_1 - c_1^\dagger c_2^\dagger - c_2^\dagger c_3 - c_3^\dagger c_2 - c_3 c_2 - c_2^\dagger c_3^\dagger). \tag{2.77}$$

Since we need to recognize the vacuum versus the excited states of $\tilde{c}$, we confirm by calculation that

$$\tilde{n}|e_s\rangle = \tilde{n}|o_s\rangle = 0 \quad \text{and} \quad \tilde{n}|e_a\rangle = 2|e_a\rangle \quad \& \quad \tilde{n}|o_a\rangle = 2|o_a\rangle, \tag{2.78}$$

concluding that the vacuum states for the $\tilde{c}$ operators are the symmetric states $|e/o_s\rangle$ while the antisymmetric states $|e/o_a\rangle$ are the excited.

Also, we can clearly see how the spectrum is doubly degenerate, split into an even parity part and odd parity part since even and odd number fermion states do not mix. In order to confirm our result, we just need to calculate how the operator $P = -i\gamma_1\gamma_6$ acts on the energy states.

2.4.4 The general N-site lattice

Continuing to work on this scheme, so generalising for the N-site arbitrary case would mean that we equip ourselves with the occupation number representation eigenstates, namely the set

of $1+\sum_{n=0}^{N}\frac{N!}{n!(N-n)!}=2^N$ eigenstates of the following table:

$\|0\rangle$		1 state
$c_i^\dagger\|0\rangle$	$1<i<N$	N states
$c_i^\dagger c_j^\dagger\|0\rangle$	$1<i<j<N$	$\frac{N(N-1)}{2!}=\frac{N!}{2!(N-2)!}$ states
$c_i^\dagger c_j^\dagger c_k^\dagger\|0\rangle$	$1<i<j<k<N$	$\frac{N(N-1)(N-2)}{3!}=\frac{N!}{3!(N-3)!}$ states
$\vdots$	$\vdots$	$\vdots$
$\prod_{i_n=1}^{m} c_{i_n}^\dagger\|0\rangle$	$1<i_1<\ldots<i_m<N$	$\frac{N(N-1)(N-2)\ldots(N-(m+1))}{m!}=\frac{N!}{m!(N-m)!}$ states
$\vdots$	$\vdots$	$\vdots$
$\prod_{i_n=1}^{N-1} c_{i_n}^\dagger\|0\rangle$	$1<i_1<\ldots<i_{N-1}<N$	$\frac{N!}{(N-1)!(N-(N-1))!}=N$ states
$\prod_{i_n=1}^{N} c_{i_n}^\dagger\|0\rangle$	$1<i_1<\ldots<i_N<N$	$\frac{N!}{N!(N-N)!}=1$ state

Those span the N-dimensional Fock space $\mathcal{F}^N=\bigoplus_{n=0}^{N}\mathcal{H}^n$, on which we find the matrix representation of the Hamiltonian (2.1) and diagonalize it. That way we can recognise the full spectrum or eigenvalues and eigenvectors for the N-site lattice. But, as the matrix of the Hamiltonian is a 2^N-dimensional matrix, tedious calculations build up.

Instead will are going to follow a different route. If we could just know the ground state of the Hamiltonian (2.1) and this happened to be the vacuum state for the $\tilde{c}$ operators, then the whole spectrum for the "refermioned" diagonal Hamiltonian of eq.(2.42) could be constructed by applying the $\tilde{c}$ operators successively. The 2-site and 3-sites problem have already shown that the ground state is symmetric and degenerate concerning parity, so following that "scent" we can guess that the ground state of even and odd parity respectively is

$$\frac{1}{\sqrt{2^N}}\sum_{n=0}^{N}\left\{\sum_{\substack{i_1\neq i_2\neq\ldots\\ \ldots\neq i_n=1}}^{n}\right\}\prod_{m=1}^{n}c_{i_m}^\dagger|0\rangle=\begin{cases}|e_s\rangle & for \quad N=N_e=2n:n\in\mathbb{N}\\ |o_s\rangle & for \quad N=N_o=2n+1:n\in\mathbb{N}\end{cases}, \tag{2.79}$$

while $N_e+N_o=N_s$ while still N_s is the number of sites.

Using eq.(2.42) we define the occupation number operator $\tilde{n}$ for the quasi-fermions created by the $\tilde{c}^\dagger$ operators, as

$$\tilde{n}=\frac{N_s-1}{2}-\frac{1}{2}\sum_{i=1}^{N_s-1}\left(c_i^\dagger c_{i+1}+c_{i+1}^\dagger c_i-c_ic_{i+1}-c_{i+1}^\dagger c_i^\dagger\right), \tag{2.80}$$

since according to eq.(2.42)

$$\begin{aligned}H=&2t\sum_{i=1}^{N_s-1}\left(\tilde{n}_i-\frac{1}{2}\right)=2t\left(\sum_{i=1}^{N_s-1}\tilde{n}_i-\frac{N_s-1}{2}\right)=2t\left(\tilde{n}-\frac{N_s-1}{2}\right)\overset{(2.1)}{\Longrightarrow}\\ \overset{(2.1)}{\Longrightarrow}\quad&\tilde{n}=\frac{N_s-1}{2}-\frac{1}{2}\sum_{i=1}^{N_s-1}\left(c_i^\dagger c_{i+1}+c_{i+1}^\dagger c_i-c_ic_{i+1}-c_{i+1}^\dagger c_i^\dagger\right).\end{aligned} \tag{2.81}$$

Applying it on the "scent" discovered ground state $|e/o_s\rangle$, we do confirm that $\tilde{n}\,|e/o_s\rangle = 0$, as

$$\left(\frac{N_s-1}{2} - \frac{1}{2}\sum_{i=1}^{N_s-1}\left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i - c_i c_{i+1} - c_{i+1}^\dagger c_i^\dagger\right)\right)\sum_{n=1}^{N}\left\{\sum_{\substack{i_1\neq i_2\neq \dots \\ \dots \neq i_n=1}}^{n}\right\}\prod_{m=1}^{n} c_{i_m}^\dagger|0\rangle\,,$$

where we can see that the action of the term $c_{i+1}^\dagger c_i^\dagger$ is compensated by the action of $c_i c_{i+1}$ and this is happening for $N_s - 1$ times due to the summation included in $\tilde{n}$. Equivalently, it happens for the $c_i^\dagger c_{i+1}$ and $c_{i+1}^\dagger c_i$ terms, leading to a zero result.

Chapter 3

Kitaev's wire coupled to fermionic baths

So far, we dealt with the $1D$ lattice of Kitaev's Hamiltonian, introduced by eq.(2.1), but haven't showed nor calculated any of its thermodynamic properties except for the energy spectrum. The question that could naturally rise would be about the behaviour of Kitaev's $1D$ lattice model in interaction with the environment. Taking the $1D$ lattice out of isolation means bringing it into contact with a bath of fermions in equilibrium, such that the $1D$ lattice microstates belong to the grand-canonical ensemble. Subsequently, finding out the Green's functions of the system would enable us to understand the system's response and calculate any of its thermodynamic and non-equilibrium quantities.

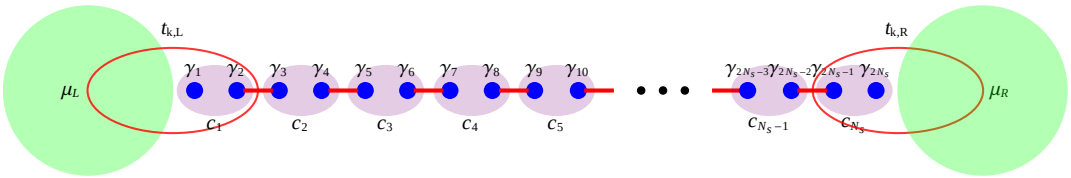

Figure 3.1: The Kitaev lattice model coupled to Fermi gas reservoirs of chemical potential $\mu_{L/R}$.

Simply, we couple our $1D$ lattice to ideal leads, see fig.3, modelled as Fermi liquid reservoirs of different chemical potentials $\mu_{L/R}$, one on each end of the lattice. The corresponding Hamiltonian of the system is

$$H_s = H_L + H_L^{cpl} + H + H_R^{cpl} + H_R\,, \tag{3.1}$$

consisting of the Hamiltonian for the Kitaev $1D$ lattice H, the ideal leads $H_{L/R}$ and the the cou-

pling between them $H_{cpl} = H_L^{cpl} + H_R^{cpl}$. They are given by

$$H = -\mu \sum_{i=1}^{N_s} n_i - \sum_{i=1}^{N_s-1} \left[t \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right) - \Delta \left(c_i c_{i+1} + c_{i+1}^\dagger c_i^\dagger \right) \right], \tag{3.2}$$

$$H_{L/R} = -\mu_{L/R} N_{L/R} + \sum_k \varepsilon_{k,L/R} c_{k,L/R}^\dagger c_{k,L/R}, \tag{3.3}$$

$$H_{cpl} = -t_{k,L} \left(c_1^\dagger c_{k,L} + c_{k,L}^\dagger c_1 \right) - t_{k,R} \left(c_{N_s}^\dagger c_{k,R} + c_{k,R}^\dagger c_{N_s} \right), \tag{3.4}$$

where $N_{L/R}$ is the number of particles in the left/right reservoir, $t_{k,L/R}$ is the hopping amplitude of the coupling between the $1D$ lattice and the left/right reservoirs, $c_{k,L/R}^\dagger / c_{k,L/R}$ are the creation/annihilation operators of particles with momentum k in the left/right reservoir and $\varepsilon_{k,L/R}$ are their energies.

3.1 A finite temperature path integral

We consider the system in equilibrium, so naturally we wish to write the partition function of the system as a path-integral of non-zero temperature in the grand-canonical ensemble. Specifically, we are interested in the sum

$$Z = \sum_n \langle n | e^{-\beta H_s} | n \rangle \tag{3.5}$$

over the complete set of Fock states $|n\rangle$ of the total system. Since this is not a convenient basis, we turn the representation of eq.(3.5) into the fermionic coherent states basis

$$Z = \int D[\psi_i^\dagger, \psi_i, \psi_{L,R}^\dagger, \psi_{L,R}] e^{-S_s[\psi_i^\dagger, \psi_i, \psi_{L,R}^\dagger, \psi_{L,R}]}, \tag{3.6}$$

where $\hbar = 1$ and the action dependent on the field $\psi = \psi(\tau)$[1]. Now, τ is the inverse temperature, while the action $S_s[\psi_i^\dagger, \psi_i, \psi_{L,R}^\dagger, \psi_{L,R}]$ consists of the sum

$$S_s[\psi_i^\dagger, \psi_i, \psi_{L,R}^\dagger, \psi_{L,R}] = S[\psi_i^\dagger, \psi_i] + S_{cpl}[\psi_i^\dagger, \psi_i, \psi_{L,R}^\dagger, \psi_{L,R}] + S_{L,R}[\psi_{L,R}^\dagger, \psi_{L,R}]. \tag{3.7}$$

The respective constituent actions are

$$S[\psi_i^\dagger, \psi_i] = \int_0^\beta d\tau \left(\sum_{i=1}^{N_s} \psi_i^\dagger \left(\partial_\tau - \mu \right) \psi_i - \sum_{i=1}^{N_s-1} \left[t \left(\psi_i^\dagger \psi_{i+1} + \psi_{i+1}^\dagger \psi_i \right) - \Delta \left(\psi_i \psi_{i+1} + \psi_{i+1}^\dagger \psi_i^\dagger \right) \right] \right), \tag{3.8}$$

$$S_{L,R}[\psi_{L,R}^\dagger, \psi_{L,R}] = \int_0^\beta d\tau \left(-\frac{1}{V} \sum_k \psi_{k,L}^\dagger \left(\partial_\tau + \varepsilon_{k,L} - \mu_L \right) \psi_{k,L} + (L \to R) \right), \tag{3.9}$$

$$S_{cpl}[\psi_i^\dagger, \psi_i, \psi_{L,R}^\dagger, \psi_{L,R}] = \int_0^\beta d\tau \left(\sum_k \frac{-t_{k,L}}{\sqrt{V}} \left(\psi_1^\dagger \psi_{k,L} + \psi_{k,L}^\dagger \psi_1 \right) + \begin{pmatrix} L \to R \\ 1 \to N_s \end{pmatrix} \right), \tag{3.10}$$

where the index k signals the momentum dependence of the coupled leads, represented by Fermi liquid reservoirs of volume V. Before plugging the action eq.(3.7) into the path integral of

[1] In the ongoing text the τ-dependance is suppressed from notation for convenience and restored where it is necessary.

eq.(3.6) and performing the calculation, I will complete the square of the action, such that using shorthand notation

$$S_{L,R}[\psi^\dagger_{L,R},\psi_{L,R}] = \int_0^\beta d\tau\Bigg\{ -\frac{1}{V}\sum_{k,k'}\psi^\dagger_{k,L}\underbrace{\left(\left(\partial_\tau+\varepsilon_{k,L}-\mu_L\right)\delta_{k,k'}\right)}_{G^{-1}_{k,k',L}}\psi_{k',L}+(L\to R)\Bigg\} \tag{3.11}$$

$$S_{L,R} = -\left(\psi_L\middle|G_L^{-1}\middle|\psi_L\right)-\left(\psi_R\middle|G_R^{-1}\middle|\psi_R\right), \tag{3.12}$$

$$S_{cpl}[\psi_i^\dagger,\psi_i,\psi^\dagger_{L,R},\psi_{L,R}] = \int_0^\beta d\tau\Bigg\{ -\frac{1}{\sqrt{V}}\sum_k t_{k,L}\left(\psi_1^\dagger\psi_{k,L}+\psi^\dagger_{k,L}\psi_1\right)+\begin{pmatrix} L\to R \\ 1\to N_s\end{pmatrix}\Bigg\} \tag{3.13}$$

$$S_{cpl} = -\left(\psi_1 t_L\middle|\psi_L\right)-\left(\psi_L\middle|t_L\psi_1\right)-\left(\psi_{N_s}t_R\middle|\psi_R\right)-\left(\psi_R\middle|t_R\psi_{N_s}\right) \tag{3.14}$$

and their sum equals

$$S_{L,R}+S_{cpl} = -\left(\psi_L+t_L\psi_1 G_L\middle|G_L^{-1}\middle|\psi_L+t_L G_L\psi_1\right)+\left(\psi_1|t_L|^2\middle|G_L\psi_1\right)+\begin{pmatrix} L\to R \\ 1\to N_s\end{pmatrix}. \tag{3.15}$$

Integrating out the fields $\psi^\dagger_{L/R},\psi_{L/R}$ in eq.(3.6) while taking into account eq.(3.15) results in

$$Z = \int D[\psi_i^\dagger,\psi_i]\, e^{-S[\psi_i^\dagger,\psi_i]-\left(\psi_1|t_L|^2\middle|G_L\psi_1\right)-\left(\psi_{N_s}|t_R|^2\middle|G_R\psi_{N_s}\right)} \tag{3.16}$$

$$= \int D[\psi_i^\dagger,\psi_i]\, e^{-S[\psi_i^\dagger,\psi_i]-\int_0^\beta d\tau\left(\psi_1^\dagger\psi_1\frac{1}{V}\sum_k|t_{k,L}|^2G_{k,L}+\psi^\dagger_{N_s}\psi_{N_s}\frac{1}{V}\sum_k|t_{k,R}|^2G_{k,R}\right)} \tag{3.17}$$

showing an effective action expression

$$S_{eff}[\psi_i^\dagger,\psi_i] = \int_0^\beta d\tau\Bigg\{\sum_{i=1}^{N_s}\psi_i^\dagger\left(\partial_\tau-\mu\right)\psi_i-\sum_{i=1}^{N_s-1}\left[t\left(\psi_i^\dagger\psi_{i+1}+\psi^\dagger_{i+1}\psi_i\right)-\Delta\left(\psi_i\psi_{i+1}+\psi^\dagger_{i+1}\psi_i^\dagger\right)\right]$$
$$-\psi_1^\dagger\psi_1\underbrace{\frac{1}{V}\sum_k|t_{k,L}|^2G_{k,L}}_{-\Sigma_L}-\psi^\dagger_{N_s}\psi_{N_s}\underbrace{\frac{1}{V}\sum_k|t_{k,R}|^2G_{k,R}}_{-\Sigma_R}\Bigg\}. \tag{3.18}$$

Defining the left/right reservoir self-energies as $\Sigma_{L/R}=\frac{1}{V}\sum_k|t_{k,L/R}|^2G_{k,L/R}$ allows us to recast it in the form

$$S_{eff}[\psi_i^\dagger,\psi_i] = \sum_{i,j=1}^{N_s}\int_0^\beta d\tau\left(\psi_i^\dagger G_{ij}^{-1}\psi_j\right), \tag{3.19}$$

where the functions noted by $G_{ij}^{\pm1}$ represent Green's functions and their inverses, obeying the defining equation

$$G_{ia}^{-1}\cdot G_{aj} = \hat{1}\Leftrightarrow\sum_a\int d\tau'' G_{ia}^{-1}(\tau-\tau'')G_{aj}(\tau''-\tau') = \delta_{ij}\delta(\tau-\tau'). \tag{3.20}$$

3.1.1 A reservoir's self-energy

At this moment let us pause to investigate the expression of self-energy $\Sigma_{L/R}$ in an extensive way. Since this is included in the inverse Green's function of the the effective action $S_{eff}[\psi_i^\dagger,\psi_i]$,

eq.(3.19), we should have established a form for it. The reservoirs are homogenous fermi gas containers of energy

$$\varepsilon_{k_{L/R}} + \varepsilon_{L/R} = \frac{{k_{L/R}}^2}{2m} + \varepsilon_{L/R},$$

where $\varepsilon_{L/R}$ is the ground state energy of each L/R reservoir respectively. Looking back at $S_{L/R}[\psi^\dagger_{L/R}, \psi_{L/R}]$ in eq.(3.11), we firstly strip it of the L/R indices such that $S_{L/R}[\psi^\dagger_{L/R}, \psi_{L/R}] = S[\psi^\dagger, \psi]$, specifically

$$S[\psi^\dagger, \psi] = -\frac{1}{V}\sum_k \int_0^\beta d\tau \left(\psi^\dagger_k(\tau)\left(\partial_\tau + \varepsilon_k + \varepsilon - \mu\right)\psi_k(\tau)\right) \tag{3.21}$$

and then we implement the Matsubara expansion for the fields

$$\psi_k(\tau) = \frac{1}{\sqrt{\beta}}\sum_n \psi_{k,n} e^{-i\omega_n \tau} \quad \text{for} \quad n = \frac{(2n+1)\pi}{\beta}. \tag{3.22}$$

Performing the Fourier integrals and summations results in

$$S[\psi^\dagger, \psi] = -\frac{1}{\beta V}\sum_{n,k} \psi^\dagger_{k,n} \underbrace{\left(-i\omega_n + \varepsilon_k + \varepsilon - \mu\right)}_{G_k^{-1}(i\omega_n)} \psi_{k,n}. \tag{3.23}$$

In section 3.1, the final step to the effective action of eq.(3.18) was performing the integrals over the fields $\psi^\dagger_{L,R}, \psi_{L,R}$. There we concluded in self-energy expressions $\Sigma_{L/R}$ involving the non-interacting Fermi gas Green's function $G_{k,L/R}$ which can now recognise as $G_{k,L/R}(i\omega_n) = -\left(-i\omega_n + \varepsilon_k + \varepsilon_{L/R} - \mu_{L/R}\right)^{-1}$, in accordance to [5], eq.(7.57). Subsequently, the self-energy expressions $\Sigma_{L/R}(i\omega_n)$ are given by

$$\Sigma_{L/R}(i\omega_n) = -\frac{1}{V}\sum_k |t_{k,L/R}|^2 G_{k,L/R}(i\omega_n) = \frac{1}{V}\sum_k \frac{|t_{k,L/R}|^2}{-i\omega_n + \varepsilon_k + \varepsilon_{L/R} - \mu_{L/R}}. \tag{3.24}$$

In order to calculate the above-mentioned expression, the summations are represented by D-dimensional integrals over momentum space. Therefore they could in general be infrared or ultraviolet divergent depending on the form of $t_{k,L/R}$ and the dimension D, they require the implementation of renormalisation techniques. In such a case we would prefer to perform the following decomposition

$$\Sigma_{L/R}(i\omega_n) = \frac{1}{V}\left(\sum_k |t_{k,L/R}|^2 \left(\frac{1}{-i\omega_n + \varepsilon_k + \varepsilon_{L/R} - \mu_{L/R}} - \frac{1}{\varepsilon_k + \varepsilon_{L/R}}\right) + \sum_k \frac{|t_{k,L/R}|^2}{\varepsilon_k + \varepsilon_{L/R}}\right) \tag{3.25}$$

and proceed to a suitable renormalisation scheme.

For our purposes, considering $t_{k,L/R} = t_{L/R} = const$ and $D = 3$, such that $\varepsilon_k \propto k^2$ will require the introduction of an ultraviolet cut-off Λ for eq.(3.24), such that it turns to the integral

$$\int_0^\Lambda dk \frac{k^2}{-i\omega_n + \varepsilon_{L/R} - \mu_{L/R} + k^2} = \left(\Lambda - \sqrt{-i\omega_n + \varepsilon_{L/R} - \mu_{L/R}}\tan^{-1}\left(\frac{\Lambda}{\sqrt{-i\omega_n + \varepsilon_{L/R} - \mu_{L/R}}}\right)\right). \tag{3.26}$$

Subsequently, if we use equation eq.(3.25) in combination with eq.(3.26) and take the limit for $\Lambda \to +\infty$ the renormalised self-energy $\Sigma^r_{L/R}(i\omega_n) = \left(\Sigma_{L/R}(i\omega_n) - \sum_k \frac{|t_{k,L/R}|^2}{\varepsilon_k + \varepsilon_{L/R}}\right)$ is

$$\Sigma^r_{L/R}(i\omega_n) = \frac{\pi}{2V}|t_{L/R}|^2\left(\sqrt{\varepsilon_{L/R}} - \sqrt{-i\omega_n + \varepsilon_{L/R} - \mu_{L/R}}\right). \tag{3.27}$$

3.2 The Green's functions

Seeking the exact form for the Green's functions for a superconducting system makes us employ the $2N_s-$dimensional Nambu space basis for the effective action given in eq.(3.19). The coherent states basis vector in the $2N_s-$dimensional Nambu space is

$$\psi_i = \left(\psi_1, \psi_2, \psi_3, \dots, \psi_{N_s-1}, \psi_{N_s}, \psi_1^\dagger, \psi_2^\dagger, \psi_3^\dagger, \dots, \psi_{N_s-1}^\dagger, \psi_{N_s}^\dagger\right)^\mathsf{T}, \tag{3.28}$$

such that the inverse Green's function takes the block form

$$G_{ij}^{-1} = \frac{1}{2}\begin{pmatrix} G_0^{-1} & \Delta \\ -\Delta & -\left(G_0^{-1}\right)^\dagger \end{pmatrix}_{ij}. \tag{3.29}$$

The block constituent $G_0^{-1} = G_{0;ij}^{-1}$ where now $i, j = 1, 2 \dots N_s$, is given by

$$G_{0;ij}^{-1} = \begin{pmatrix} (\partial_\tau - \mu) + \Sigma_L & -t & 0 & \dots & \dots & 0 \\ -t & (\partial_\tau - \mu) & -t & 0 & \dots & 0 \\ 0 & -t & \ddots & \ddots & 0 & \vdots \\ \vdots & 0 & \ddots & \ddots & -t & 0 \\ 0 & \dots & 0 & -t & (\partial_\tau - \mu) & -t \\ 0 & \dots & \dots & 0 & -t & (\partial_\tau - \mu) + \Sigma_R \end{pmatrix} \tag{3.30}$$

and happens to be equal to the Green's function G_{ij}^{-1} for the case of $\Delta = 0$; while the other block N_s-dimensional constituent $\Delta = \Delta_{ij}$ incorporates the superconducting behaviour of the system, being

$$\Delta = \Delta_{ij} = \begin{pmatrix} 0 & \Delta & 0 & \dots & \dots & 0 \\ -\Delta & 0 & \Delta & 0 & \dots & 0 \\ 0 & -\Delta & \ddots & \ddots & 0 & \vdots \\ \vdots & 0 & \ddots & \ddots & \Delta & 0 \\ 0 & \dots & 0 & -\Delta & 0 & \Delta \\ 0 & \dots & \dots & 0 & -\Delta & 0 \end{pmatrix}. \tag{3.31}$$

A paradigm. The Green's function for a 2-site lattice.

Having established a method for the calculation of the system's equilibrium Green's function G_{ij} and an expression for the self-energies $\Sigma_{L/R}$, let us demonstrate their explicit form for the 2-site lattice as an illustrative example. The inverse Green's functions have the matrix form

$$G_{ij}^{-1} = \frac{1}{2}\begin{pmatrix} G_0^{-1} & \Delta \\ -\Delta & -\left(G_0^{-1}\right)^\dagger \end{pmatrix}_{ij}, \text{ where } \quad G_{0;ij}^{-1} = \begin{pmatrix} (\partial_\tau - \mu) + \Sigma_L & -t \\ -t & (\partial_\tau - \mu) + \Sigma_R \end{pmatrix}$$

$$\text{or} \qquad G_{ij}^{-1} = \frac{1}{2}\begin{pmatrix} (\partial_\tau - \mu) + \Sigma_L & -t & 0 & \Delta \\ -t & (\partial_\tau - \mu) + \Sigma_R & -\Delta & 0 \\ 0 & -\Delta & (\partial_\tau + \mu) - \Sigma_L & +t \\ \Delta & 0 & +t & (\partial_\tau + \mu) - \Sigma_R \end{pmatrix}, \tag{3.32}$$

while the Green's functions are given by

$$G_{ia}^{-1}\cdot G_{aj}=\hat{\mathbf{1}}\Leftrightarrow\sum_{a}\int d\tau''\,G_{ia}^{-1}(\tau-\tau'')\,G_{aj}(\tau''-\tau')=\delta_{ij}\delta(\tau-\tau'). \tag{3.33}$$

Expanding $G_{aj}(\tau''-\tau')$ and $\Sigma_{L/R}(\tau)$ over Matsubara fermionic frequencies[2] $\omega_n=\frac{(2n+1)\pi}{\beta}$, for $n\in\mathbb{Z}$, results in the following equation

$$\frac{1}{2}\begin{pmatrix}G_0^{-1}(i\omega_n) & \Delta\\ -\Delta & -\left(G_0^{-1}\right)^{\dagger}(i\omega_n)\end{pmatrix}_{ia}\cdot G_{aj}(i\omega_n)=\delta_{ij}\,, \tag{3.34}$$

where

$$G_0^{-1}(i\omega_n)=\begin{pmatrix}i\omega_n-\mu+\Sigma_L & -t\\ -t & i\omega_n-\mu+\Sigma_R\end{pmatrix} \tag{3.35}$$

and

$$-\left(G_0^{-1}\right)^{\dagger}(i\omega_n)=\begin{pmatrix}i\omega_n+\mu-\Sigma_L^{\dagger} & +t\\ +t & i\omega_n+\mu-\Sigma_R^{\dagger}\end{pmatrix}. \tag{3.36}$$

This is solved by

$$G_{ij}(\tau)=\sum_{n}\frac{\frac{e^{-i\omega_n\tau}}{2}}{\left(\left(-i\omega_n-\mu+\Sigma_L(i\omega_n)\right)\left(-i\omega_n-\mu+\Sigma_R(i\omega_n)\right)-t^2+\Delta^2\right)^2}\begin{pmatrix}\mathcal{G}_0 & \Delta\\ -\Delta & -\left(\mathcal{G}_0\right)^{\dagger}\end{pmatrix}_{ij}, \tag{3.37}$$

while $\mathcal{G}_0=\begin{pmatrix}-i\omega_n-\mu+\Sigma_R(i\omega_n) & t\\ t & -i\omega_n-\mu+\Sigma_L(i\omega_n)\end{pmatrix}$.

[2]Note that the expansion for the G_0^{-1} block component is $\int d\tau''\,G_0^{-1}(\tau-\tau'')G_0^{-1}(\tau''-\tau')=\delta_{ij}\delta(\tau-\tau')\Rightarrow$

$\Rightarrow\int d\tau''\begin{pmatrix}(\partial_\tau-\mu)\delta(\tau-\tau'')+\Sigma_L(\tau-\tau'') & -t\delta(\tau-\tau'')\\ -t\delta(\tau-\tau'') & (\partial_\tau-\mu)\delta(\tau-\tau'')+\Sigma_R(\tau-\tau'')\end{pmatrix}\sum_n G_{0;aj}(i\omega_n)\,e^{-i\omega_n(\tau''-\tau')}=\delta_{ij}\delta(\tau-\tau')\Rightarrow$

$\Rightarrow\begin{pmatrix}-i\omega_n-\mu+\Sigma_L(i\omega_n) & -t\\ -t & -i\omega_n-\mu+\Sigma_R(i\omega_n)\end{pmatrix}\cdot G_{0;aj}(i\omega_n)=\delta_{ij}$

.

Chapter 4

Out of equilibrium considerations

Until this point all our methods were based on the assumption that the system had been given enough time to relax to a *"Thermodynamic Equilibrium"* state, such that

> *The isolated system is characterised by a unique set of time-independant extensive and intensive variables*

or a *"Stationary Thermodynamic Non-Equilibrium"* state, under which

> *The system is characterised by a unique set of time-independant extensive and intensive variables, under the condition that the environment remains unchanged.*

The system setup introduced in chapter 3 includes an $1D$ lattice, while the environment consists of Fermi liquid reservoirs coupled to it. In the previous section 3.2 we showed how the reservoirs can be integrated out of the path integral and included in the equilibrium Green's functions as self-energy terms $\Sigma_{L/R}$. In this chapter we treat the same setup, characterised by a Hamiltonian like the one of eq.(3.1) but in a non-equilibrium way. We aim to calculate the conductivity of Kitaev's lattice model due to the chemical potential differences for the reservoirs. But since a current flow J is a non-equilibrium quantity, we need to employ non-equilibrium Green's functions instead of the equilibrium ones of the previous chapter.

4.1 Langevin Equations

Motivated by the previous chapter's equilibrium approach, where we calculated the Green's functions and showed how the reservoir's effect is included as self-energies $\Sigma_{L/R}$, we will mount directly on the non-equilibrium approach starting from the equations of motion. The setup of the system is given by a type of Hamiltonian like the one of eq.(3.1), but since the system is no longer in equilibrium a path-integral over the inverse temperature $\tau = -i\beta$ - like the one of eq.(3.5) - cannot be written. So, let us just consider reservoirs that are large enough in comparison to the $1D$ lattice such that are in equilibrium while they produce and propagate noise within the $1D$ lattice wire.

The system consists of a N-site $1D$ lattice having chemical potential μ, characterised by the fermionic fields $\psi_i(\tau), \psi_i^\dagger(\tau)$[1] and coupled with Fermi gas reservoirs in equilibrium, while these

[1] Please note that τ is no more the inverse temperature of the previous chapter but ordinary time. The Greek character τ is used instead of the usual t since this was reserved for the hoping parameter.

are identified by different chemical potentials $\mu_{1/2} = \mu_{L/R}$. The reservoirs are characterised by and coupled to the lattice by means of self-energies $\Sigma^{+}_{L/R}(\tau-\tau')$, $\Sigma^{-}_{L/R}(\tau'-\tau)$ - the retarded and advanced respectively - while they are also responsible for noise in the system, characterised by the functions $\eta_{L/R}(\tau)$, $\eta^{\dagger}_{L/R}(\tau)$. Of course each of the retarded/advanced self-energies, in order to justify its name, incorporates the Heaviside function $\Theta(\pm(\tau-\tau'))$ respectively. The system is dictated by the following Langevin equations

$$\left(i\hbar\frac{\partial}{\partial\tau}-\mu\right)\psi_i(\tau)-\int_{-\infty}^{+\infty}d\tau'\hbar S^{+}_{ij}(\tau-\tau')\,\psi_j(\tau')=\eta_i(\tau), \tag{4.1a}$$

$$\left(-i\hbar\frac{\partial}{\partial\tau}-\mu\right)\psi^{\dagger}_i(\tau)-\int_{-\infty}^{+\infty}d\tau'\psi^{\dagger}_j(\tau')\,\hbar S^{-}_{ji}(\tau'-\tau)=\eta^{\dagger}_i(\tau), \tag{4.1b}$$

where repeated indices are summed over. Implementing the Nambu base for the fermion's field

$$\psi_i(\tau)=\left(\psi_1(\tau),\,\ldots,\psi_{N-1}(\tau),\psi_N(\tau),\psi^{\dagger}_1(\tau),\ldots,\psi^{\dagger}_{N-1}(\tau),\psi^{\dagger}_N(\tau)\right)^{\mathsf{T}} \tag{4.2}$$

and the noise field

$$\eta_i(\tau)=\left(\eta_L(\tau),0,\ldots,0,\eta_R(\tau),\eta^{\dagger}_L(\tau),0,\ldots,0,\eta^{\dagger}_R(\tau)\right)^{\mathsf{T}}, \tag{4.3}$$

results in

$$\hbar S^{+}_{ij}(\tau-\tau')=\frac{1}{2}\begin{pmatrix}\hbar S^{+}_0(\tau-\tau') & \Delta\\ -\Delta & -\hbar S^{-}_0(\tau'-\tau)\end{pmatrix}_{ij}. \tag{4.4}$$

The matrix Δ is given by eq.(3.31) like in section 3.2 and

$$\hbar S^{+}_{0;ij}=\begin{pmatrix}\hbar\Sigma^{+}_L(\tau-\tau') & -t\,\delta(\tau-\tau') & 0 & \ldots & \ldots & 0\\ -t\,\delta(\tau-\tau') & 0 & -t\,\delta(\tau-\tau') & 0 & \ldots & 0\\ 0 & -t\,\delta(\tau-\tau') & \ddots & \ddots & 0 & \vdots\\ \vdots & 0 & \ddots & \ddots & -t\,\delta(\tau-\tau') & 0\\ 0 & \ldots & 0 & -t\,\delta(\tau-\tau') & 0 & -t\,\delta(\tau-\tau')\\ 0 & \ldots & \ldots & 0 & -t\,\delta(\tau-\tau') & \hbar\Sigma^{+}_R(\tau-\tau')\end{pmatrix},$$

while $S^{+}_{ij}(\tau-\tau')$ is symmetric and $S^{+}_{ij}(\tau-\tau')=\left(S^{-}_{ji}(\tau'-\tau)\right)^{\dagger}$.

4.2 The non-equilibrium Green's functions

According to the definitions given for our system, we recognise the inverse retarded Green's function as

$$G^{+^{-1}}_{ij}(\tau-\tau')=-\frac{1}{\hbar}\left(\left(i\hbar\frac{\partial}{\partial\tau}-\mu\right)\delta_{ij}\,\delta(\tau-\tau')-\hbar S^{+}_{ij}(\tau-\tau')\right), \tag{4.5}$$

which satisfies the usual defining relation

$$\int_{-\infty}^{+\infty}d\tau''\,G^{+^{-1}}_{ia}(\tau-\tau'')\cdot G^{+}_{aj}(\tau''-\tau')=\delta_{ij}\,\delta(\tau-\tau'), \tag{4.6}$$

while $G_{ia}^{+^{-1}}(\tau-\tau') = \left(G_{ia}^{-^{-1}}(\tau'-\tau)\right)^{\dagger}$.

As a first step we implement Fourier transformations, which will prove to be handy later on, so by defining the transformation for the fields as

$$\psi_i(\tau) = \int_{-\infty}^{+\infty} \frac{dE}{\sqrt{2\pi\hbar}} \psi_i(E) e^{-i\frac{E}{\hbar}\tau}, \quad \psi_i^{\dagger}(\tau) = \int_{-\infty}^{+\infty} \frac{dE}{\sqrt{2\pi\hbar}} \psi_i^{\dagger}(E) e^{+i\frac{E}{\hbar}\tau}, \tag{4.7}$$

consequently, the Fourier transform of self-energy terms is

$$S_{ij}^{\pm}(\tau-\tau') = \int_{-\infty}^{+\infty} \frac{dE}{2\pi\hbar} S_{ij}^{\pm}(E) e^{\mp i\frac{E}{\hbar}(\tau-\tau')}, \tag{4.8}$$

where we take advantage of the symmetry over the indices in $S_{ij}^{+}(E)$ and we also recognise that $S_{ij}^{+}(E) = \left(S_{ji}^{-}(E)\right)^{\dagger} = \left(S_{ji}^{-}(E)\right)^{*}$. Lastly, the noise terms transform as

$$\eta_i(\tau) = \int_{-\infty}^{+\infty} \frac{dE}{\sqrt{2\pi\hbar}} \eta_i(E) e^{-i\frac{E}{\hbar}\tau}, \quad \eta_i^{\dagger}(\tau) = \int_{-\infty}^{+\infty} \frac{dE}{\sqrt{2\pi\hbar}} \eta_i^{\dagger}(E) e^{+i\frac{E}{\hbar}\tau}. \tag{4.9}$$

Now, plugging the above-mentioned expressions in the Langevin equations (4.1) and performing the Fourier integrals, results in the Fourier transformed equations

$$\left((E-\mu)\,\delta_{ij} - \hbar S_{ij}^{+}(E)\right) \cdot \psi_j(E) = -\hbar G_{ij}^{+^{-1}}(E) \cdot \psi_j(E) = \eta_i(E), \tag{4.10a}$$

$$\psi_j^{\dagger}(E) \cdot \left((E-\mu)\,\delta_{ji} - \hbar S_{ji}^{-}(E)\right) = \psi_j^{\dagger}(E) \cdot \left(-\hbar G_{ji}^{-^{-1}}(E)\right) = \eta_i^{\dagger}(E), \tag{4.10b}$$

for the $1D$ lattice.

Note that on eq.(4.10) I have silently introduced the inverse of the Fourier transform of the retarded/advanced Green's functions $G_{ij}^{\pm^{-1}}(E)$ which define the Green's functions $G_{ij}^{\pm}(E)$ through the relation

$$G_{ia}^{\pm^{-1}}(E) \cdot G_{aj}^{\pm}(E) = \delta_{ij} \Rightarrow \frac{\left((E-\mu)\,\delta_{ia} - \hbar S_{ia}^{\pm}(E)\right)}{-\hbar} \cdot G_{aj}^{\pm}(E) = \delta_{ij}, \tag{4.11}$$

where $G_{ia}^{\pm^{-1}}(E) = -\frac{1}{2\hbar} \begin{pmatrix} G_0^{\pm^{-1}}(E) & \Delta \\ -\Delta & -G_0^{\mp^{-1}}(-E) \end{pmatrix}_{ia}$, while $G_{0;ia}^{\pm^{-1}}(E)$ is a N_s-dimensional matrix given by

$$G_{0;ia}^{\pm^{-1}}(E) = -\frac{1}{\hbar} \begin{pmatrix} E-\mu-\hbar\Sigma_L^{\pm}(E) & -t & 0 & \dots & \dots & 0 \\ -t & E-\mu & -t & 0 & \dots & 0 \\ 0 & -t & \ddots & \ddots & 0 & \vdots \\ \vdots & 0 & \ddots & \ddots & -t & 0 \\ 0 & \dots & 0 & -t & E-\mu & -t \\ 0 & \dots & \dots & 0 & -t & E-\mu-\hbar\Sigma_R^{\pm}(E) \end{pmatrix}. \tag{4.12}$$

In order to calculate the Green's function $G_{0;ia}^{\pm}(E)$ it is handy to implement the block-wise matrix

inversion technique [2] in order to arrive at

$$G^{\pm}_{aj} = 2\hbar \begin{pmatrix} -\left(G_0^{\pm^{-1}}(E) - \Delta G_0^{\mp}(-E)\Delta\right)^{-1} & G_0^{\pm}(E)\Delta\left(-G_0^{\mp^{-1}}(-E) + \Delta G_0^{\pm}(E)\Delta\right)^{-1} \\ G_0^{\mp}(-E)\Delta\left(G_0^{\pm^{-1}}(E) - \Delta G_0^{\mp}(-E)\Delta\right)^{-1} & -\left(-G_0^{\mp^{-1}}(-E) + \Delta G_0^{\pm}(E)\Delta\right)^{-1} \end{pmatrix}_{aj}.$$

4.3 The lesser Green's function

Solving eq.(4.10) for the Fourier transformed fields $\psi_i^{\dagger}(E), \psi_j(E)$ we obtain

$$\psi_i(E) = G^{+}_{il}(E)\cdot\eta_l(E) \quad \& \quad \psi^{\dagger}_j(E) = \eta^{\dagger}_k(E)\cdot G^{-}_{kj}(E) \tag{4.15}$$

and we are able to claim that the expectation value of the correlation function of the fields is

$$\left\langle \psi_i^{\dagger}(E')\psi_j(E)\right\rangle = G^{-}_{ki}(E')\cdot\left\langle \eta_k^{\dagger}(E')\eta_l(E)\right\rangle\cdot G^{+}_{jl}(E). \tag{4.16}$$

Equating the energies, $E = E'$ and taking into account that the Green's functions are symmetric, such that $G^{\pm}_{ij}(E) = G^{\pm}_{ji}(E)$, leads to the expectation value for the lesser Green's function $G^{<}_{ij}(E)$[3] as

$$\left\langle \psi_i^{\dagger}(E)\psi_j(E)\right\rangle = -iG^{<}_{ij}(E) = G^{-}_{ik}(E)\cdot\left\langle \eta_k^{\dagger}(E)\eta_l(E)\right\rangle\cdot G^{+}_{lj}(E)\,. \tag{4.17}$$

In order to evaluate eq.(4.17) we need to understand what the noise correlation function is. Considering that the noise comes from the reservoirs in equilibrium, we adopt the following ansatz for its correlation function

$$\left\langle \eta_k^{\dagger}(E)\eta_l(E)\right\rangle = 2\pi\hbar\left(\frac{-1}{\pi\hbar}\,\mathrm{Im}\left[\hbar S^{+}_{kl}(E)\right]\right)N_{FD}(E-(\mu_k-\mu))^{[4]} \tag{4.18}$$

and seek for its justification.

4.4 The fluctuation-dissipation theorem

The justification of the above-mentioned ansatz goes through the fluctuation-dissipation theorem which establishes the connection between a non-equilibrium state and an equilibrium one. Namely, it states that:

---

[2] An $n+n'$ dimensional matrix M, composed by the block form $M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$, where the blocks A, D are invertible square matrices of n, n' dimensions respectively and B, C are $n\times n'$, $n'\times n$ dimensional matrices respectively, is invertible and it's inverse is given by the general formula

$$M^{-1} = \begin{pmatrix} (A-BD^{-1}C)^{-1} & -A^{-1}B\left(D-CA^{-1}B\right)^{-1} \\ -D^{-1}C\left(A-BD^{-1}C\right)^{-1} & \left(D-CA^{-1}B\right)^{-1} \end{pmatrix} \tag{4.13}$$

which for $C=-B$ and $D=-A^{\dagger}$ becomes

$$M^{-1} = \begin{pmatrix} \left(A-B\left(A^{\dagger}\right)^{-1}B\right)^{-1} & -A^{-1}B\left(-A^{\dagger}+BA^{-1}B\right)^{-1} \\ -\left(A^{\dagger}\right)^{-1}B\left(A-B\left(A^{\dagger}\right)^{-1}B\right)^{-1} & \left(-A^{\dagger}+BA^{-1}B\right)^{-1} \end{pmatrix}. \tag{4.14}$$

[3] This is the Fourier transformation of the the original lesser Green's function $G^{<}_{ij}(\tau)$.

[4] Now, the repeated indices do not imply any summation.

Theorem. *Fluctuation - Dissipation (Langevin) Theorem: The equilibrium is brought about by a dissipative interaction ("friction") between the system and the reservoir. Whatever the dissipative mechanism, it is the same process that produces the random, fluctuating behaviour of the system. Moreover, both processes are uniquely determined by the statistical nature of the microscopic processes of the interaction.*

In equilibrium, for our setup, the above is translated to a relation between the lesser Green's function and the spectral function, namely

$$G_{ij}^{<}(E) = \rho_{ij} N(E) = -\frac{1}{\pi\hbar}\mathrm{Im}\left[G_{ij}^{+}(E)\right] N(E), \tag{4.19}$$

where $N(E)$ is the equilibrium distribution function - in our case the Fermi-Dirac distribution $N(E) = N_{FD}(E) = \left(1 + e^{\beta(E-\mu)}\right)^{-1}$. The relation of eq.(4.19) establishes an equilibrium initial condition for the non-equilibrium lesser function $G_{ij}^{<}(E)$. In parallel, a useful ansatz has been proposed; consider replacing the equilibrium distribution function $N(E)$ by an unknown non-equilibrium one.

Consider the situation of a single site coupled to a reservoir in equilibrium. According to our results from the previous section 4.3 for $\langle N(E)\rangle$ at the first site we should have

$$2\pi\hbar\langle N(E)\rangle = \left\langle \psi_1^{\dagger}(E)\psi_1(E)\right\rangle = -iG_{11}^{<}(E) = G_{1k}^{-}(E)\cdot\left\langle \eta_k^{\dagger}(E)\eta_l(E)\right\rangle \cdot G_{l1}^{+}(E)\Big|_{k,l=1} \Rightarrow$$

$$\langle N(E)\rangle = \frac{\hbar}{2\pi}\frac{\left\langle \eta_L^{\dagger}(E)\eta_L(E)\right\rangle}{\left(E-\mu-\hbar\Sigma_L^{-}(E)\right)\left(E-\mu-\hbar\Sigma_L^{+}(E)\right)}. \tag{4.20}$$

If we define $\Sigma_{L/R}^{\pm}(E) = \mathrm{Re}\left[\Sigma_{L/R}^{\pm}(E)\right] + i\,\mathrm{Im}\left[\Sigma_{L/R}^{\pm}(E)\right] = \Sigma_{L/R}^{\prime +}(E) \pm i\Sigma_{L/R}^{\prime\prime +}(E)$, since for the self-energies it holds that $\Sigma_{ij}^{+}(E) = \left(\Sigma_{ij}^{-}(E)\right)^{*}$, the expression for $\langle N(E)\rangle$ results in

$$\langle N(E)\rangle = \frac{\hbar}{2\pi}\frac{\left\langle \eta_L^{\dagger}(E)\eta_L(E)\right\rangle}{\left(E-\mu-\hbar\Sigma_L^{\prime +}(E)\right)^2 + \left(\hbar\Sigma_L^{\prime\prime +}(E)\right)^2}. \tag{4.21}$$

Thanks to the fluctuation-dissipation theorem - in parallel - we know that the density function in equilibrium is connected to the spectral function $\rho(E)$ as

$$\langle N(E)\rangle = \rho_{11}(E)N_{FD}(E) = -\frac{1}{\pi\hbar}\mathrm{Im}\left[G_{11}^{+}(E)\right] N_{FD}(E) = -\frac{1}{\pi\hbar}\mathrm{Im}\left[\frac{\hbar}{E-\mu-\hbar\Sigma_L^{+}(E)}\right] N_{FD}(E) \Rightarrow$$

$$\langle N(E)\rangle = \frac{1}{\pi}\frac{-\hbar\Sigma_L^{\prime\prime +}(E)N_{FD}(E)}{\left(E-\mu-\hbar\Sigma_L^{\prime +}(E)\right)^2 + \left(\hbar\Sigma_L^{\prime\prime +}(E)\right)^2}, \tag{4.22}$$

so by comparing the two expressions, eq.(4.22) and eq.(4.21), we conclude that

$$\left\langle \eta_L^{\dagger}(E)\eta_L(E)\right\rangle = -2\Sigma_L^{\prime\prime +}(E)N_{FD}(E) \tag{4.23}$$

in equilibrium. This is justifiably extended to the ansatz

$$\left\langle \eta_{L/R}^{\dagger}(E)\eta_{L/R}(E)\right\rangle = -2\Sigma_{L/R}^{\prime\prime +}(E)N_{FD}(E-(\mu_{L/R}-\mu)), \tag{4.24}$$

which is in accordance with eq.(4.18) for the correlation function of the noise.

4.4.1 The real & complex part of a reservoir's self-energy

A constituent that remains to be determined is the explicit equilibrium form of the self-energy $\Sigma^{+}(E)$, where $\Sigma^{'+}(E) = \mathrm{Re}\left[\Sigma^{+}(E)\right]$ and $\Sigma^{''+}(E) = \mathrm{Im}\left[\Sigma^{+}(E)\right]$. In accordance to section 3.1.1 and eq.(3.24) we have

$$\Sigma^{+}(E) = -\frac{t^2}{V}\sum_k G_k(E) = t^2\int_0^{+\infty}\frac{k^2}{(E+i\varepsilon)+\frac{k^2}{2m_e}-\mu+E_{k_0}}dk, \tag{4.25}$$

where $\varepsilon \to 0^{+}$. Following the Sokhotski-Plemelj theorem, see app.D, we have

$$\Sigma^{+}(E) = m_e t^2\left(-i\pi\sqrt{2m_e\left(E+E_{k_0}-\mu\right)}+\mathcal{P}\int_0^{+\infty}\frac{2k}{k^2+2m_e\left(E+E_{k_0}-\mu\right)}dk\right) \tag{4.26}$$

where $\mathcal{P}$ denotes the Cauchy principal value.

4.5 A non-equilibrium revision of the 2-site lattice

By the end of section 3.2 we calculated the explicit form of the equilibrium Green's functions for a 2-site lattice. Following that, in the current section we will calculate the non-equilibrium Green's functions. It serves as an illustrative example for the N-site case; these calculations cannot be performed by hand and shown within the borderlines of a page. After showing the non-equilibrium Green's functions we will turn to the spectral function $\rho_{ij}(E)$ and the conductivity σ.

4.5.1 The non-equilibrium Green's functions

For the 2-site lattice, the expressions of the retarded/advanced inverse Green's function are

$$G_{aj}^{\pm^{-1}}(E) = \frac{-1}{2\hbar}\begin{pmatrix} E-\mu-\hbar\Sigma_L^{\pm}(E) & -t & 0 & \Delta \\ -t & E-\mu-\hbar\Sigma_R^{\pm}(E) & -\Delta & 0 \\ 0 & -\Delta & E+\mu+\hbar\Sigma_L^{\mp}(E) & +t \\ \Delta & 0 & +t & E+\mu+\hbar\Sigma_R^{\mp}(E) \end{pmatrix}, \tag{4.27}$$

resulting in the retarded/advanced Green's function

$$G_{aj}^{\pm}(E) = -2\hbar\begin{pmatrix} \left(G_0^{\pm^{-1}}-\Delta G_0^{\mp}\Delta\right)^{-1} & -G_0^{\pm}\Delta\left(-G_0^{\mp^{-1}}+\Delta G_0^{\pm}\Delta\right)^{-1} \\ -G_0^{\mp}\Delta\left(G_0^{\pm^{-1}}-\Delta G_0^{\mp}\Delta\right)^{-1} & \left(-G_0^{\mp^{-1}}+\Delta G_0^{\pm}\Delta\right)^{-1} \end{pmatrix}_{aj}, \tag{4.28}$$

where now $G_0^{\pm^{-1}} = G_0^{\pm^{-1}}(E) = \begin{pmatrix} E-\mu-\hbar\Sigma_L^{\pm}(E) & -t \\ -t & E-\mu-\hbar\Sigma_R^{\pm}(E) \end{pmatrix}$ and $\Delta = \begin{pmatrix} 0 & \Delta \\ -\Delta & 0 \end{pmatrix}$, while of course $G_0^{\mp^{-1}} = -G_0^{\pm^{-1}}(-E)$ as before. Tedious calculations result in

$$G_{aj}^{\pm}(E) = \frac{1}{Det\left[G_{aj}^{\pm^{-1}}(E)\right]}\begin{pmatrix} \tilde{G}_{11}^{\pm}(E) & \tilde{G}_{12}^{\pm}(E) & \tilde{G}_{13}^{\pm}(E) & \tilde{G}_{14}^{\pm}(E) \\ \tilde{G}_{21}^{\pm}(E) & \tilde{G}_{22}^{\pm}(E) & \tilde{G}_{23}^{\pm}(E) & \tilde{G}_{24}^{\pm}(E) \\ \tilde{G}_{31}^{\pm}(E) & \tilde{G}_{32}^{\pm}(E) & \tilde{G}_{33}^{\pm}(E) & \tilde{G}_{34}^{\pm}(E) \\ \tilde{G}_{31}^{\pm}(E) & \tilde{G}_{42}^{\pm}(E) & \tilde{G}_{43}^{\pm}(E) & \tilde{G}_{44}^{\pm}(E) \end{pmatrix}, \tag{4.29}$$

where

$$\begin{aligned}
\tilde{G}^{\pm}_{11}(E) =& \frac{1}{8\hbar^3}\Big(\big(E+\mu+\hbar\Sigma^{\mp}_R(E)\big)\Big[\big(E-\mu-\hbar\Sigma^{\pm}_R(E)\big)\big(E+\mu+\hbar\Sigma^{\mp}_L(E)\big)+\Delta^2\Big] \\
&-t^2\big(E-\mu-\hbar\Sigma^{\pm}_R(E)\big)\Big), \\
\tilde{G}^{\pm}_{12}(E) =& G^{\pm}_{21}(E) = \frac{t}{8\hbar^3}\big(t^2-\Delta^2-\big(E+\mu+\hbar\Sigma^{\mp}_L(E)\big)\big(E+\mu+\hbar\Sigma^{\mp}_R(E)\big)\big), \\
\tilde{G}^{\pm}_{22}(E) =& \frac{1}{8\hbar^3}\Big(\big(E+\mu+\hbar\Sigma^{\mp}_L(E)\big)\Big[\big(E-\mu-\hbar\Sigma^{\pm}_L(E)\big)\big(E+\mu+\hbar\Sigma^{\mp}_R(E)\big)+\Delta^2\Big] \\
&-\big(E-\mu-\hbar\Sigma^{\pm}_L(E)\big)t^2\Big), \\
\tilde{G}^{\pm}_{13}(E) =& \tilde{G}^{\pm}_{31}(E) = -\frac{2t\Delta}{8\hbar^3}\big(E-i\hbar\,\mathrm{Im}\big[\Sigma^{\pm}_R(E)\big]\big), \\
\tilde{G}^{\pm}_{14}(E) =& \tilde{G}^{\pm}_{41}(E) = \frac{\Delta}{8\hbar^3}\big(t^2-\Delta^2-\big(E-\mu-\hbar\Sigma^{\pm}_R(E)\big)\big(E+\mu+\hbar\Sigma^{\mp}_L(E)\big)\big), \\
\tilde{G}^{\pm}_{23}(E) =& \tilde{G}^{\pm}_{32}(E) = \frac{-\Delta}{8\hbar^3}\big(t^2-\Delta^2-\big(E-\mu-\hbar\Sigma^{\pm}_L(E)\big)\big(E+\mu+\hbar\Sigma^{\mp}_R(E)\big)\big), \\
\tilde{G}^{\pm}_{24}(E) =& \tilde{G}^{\pm}_{42}(E) = \frac{2t\Delta}{8\hbar^3}\big(E-i\hbar\,\mathrm{Im}\big[\Sigma^{\pm}_L(E)\big]\big), \\
\tilde{G}^{\pm}_{33}(E) =& \big(E+\mu+\hbar\Sigma^{\mp}_R(E)\big)\Big[\hbar\Sigma^{\pm}_L(E)\big(E-\mu-\hbar\Sigma^{\pm}_R(E)\big)+(E-\mu)\hbar\Sigma^{\pm}_R(E)-(E-\mu+t)(E-\mu-t)\Big] \\
&+\Delta^2\big(E-\mu-\hbar\Sigma^{\pm}_L(E)\big), \\
\tilde{G}^{\pm}_{34}(E) =& \tilde{G}^{\pm}_{43}(E) = t\big(\Delta^2-t^2+(E-\mu)^2-\hbar\Sigma^{\pm}_L(E)\big(E-\mu-\hbar\Sigma^{\pm}_R(E)\big)-(E-\mu)\hbar\Sigma^{\pm}_R(E)\big), \\
\tilde{G}^{\pm}_{44}(E) =& \big(E+\mu+\hbar\Sigma^{\mp}_L(E)\big)\Big[\hbar\Sigma^{\pm}_L(E)\big(E-\mu-\hbar\Sigma^{\pm}_R(E)\big)+(E-\mu)\hbar\Sigma^{\pm}_R(E)-(E-\mu+t)(E-\mu-t)\Big] \\
&+\Delta^2\big(E-\mu-\hbar\Sigma^{\pm}_R(E)\big),
\end{aligned}$$

while

$$\begin{aligned}
Det\Big[G^{\pm^{-1}}_{aj}(E)\Big] = \frac{1}{16\hbar^4}\Big(&\big(t^2-\Delta^2\big)^2-\Delta^2\big[\big(E-\mu-\hbar\Sigma^{\pm}_R(E)\big)\big(E+\mu+\hbar\Sigma^{\mp}_L(E)\big)+(L\to R)\big] \\
&-t^2\big[\big(E-\mu-\hbar\Sigma^{\pm}_L(E)\big)\big(E-\mu-\hbar\Sigma^{\pm}_R(E)\big)+\big(E+\mu+\hbar\Sigma^{\mp}_L(E)\big)\big(E+\mu+\hbar\Sigma^{\mp}_R(E)\big)\big] \\
&+\big(E-\mu-\hbar\Sigma^{\pm}_L(E)\big)\big(E-\mu-\hbar\Sigma^{\pm}_R(E)\big)\big(E+\mu+\hbar\Sigma^{\mp}_L(E)\big)\big(E+\mu+\hbar\Sigma^{\mp}_R(E)\big)\Big).
\end{aligned}$$

4.5.2 The spectral function

Having the Green's functions at hand enables us to calculate and plot all the quantities of interest. The spectral function $\rho_{ij}(E)$ is related to the advanced Green's function via

$$\rho_{ij}(E) = -\frac{1}{\pi\hbar}\mathrm{Im}\Big[G^{+}_{ij}(E)\Big], \tag{4.30}$$

which is a dimensionless quantity directly related to the single-particle density of states. In section 2.4.2 we calculated the energy eigenvalues for the general case of $t \neq \Delta$, so we should now expect to see the maximums of the spectral function $\rho_{11}(E)$ or $\rho_{22}(E)$ to lie at those values.

Assuming the equilibrium case where the reservoir's self-energies $\Sigma^{\pm}_L(E) = \Sigma^{\pm}_R(E) = \Sigma^{\pm}(E)$ equate, since all chemical potentials should equate $\mu_R = \mu_L = \mu$, we plot the spectral function $\rho_{11}(E) = \rho_{22}(E)$ with respect to the energy of the system E/t. The peaks of the spectral function $\rho_{11}(E)$ or $\rho_{22}(E)$ are expected to be located at the eigenenergies of the system. Recalling section

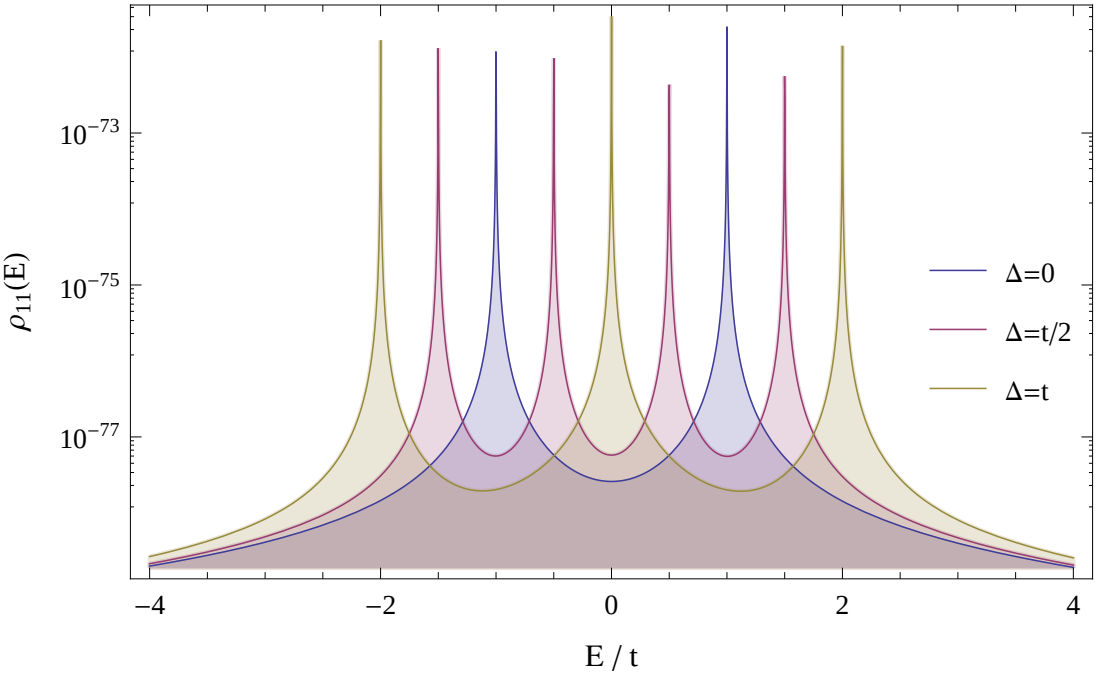

Figure 4.1: The spectral function $\rho_{ij}(E)$, plotted for $\mu = 0$ and $E_{k_0} = -100t$. The blue line $(\Delta = 0)$ shows two peaks, namely at $E = \pm t$, as is expected for the absence of superconductivity while for $(\Delta = t/2)$ we observe four peaks at $E = \pm(t \pm \Delta)$. Note that both axis are dimensionless.

2.4.2 where we solved the system in the Nambu base, reminds us that the energies for the eigenstates of the system are $E = \pm(t \pm \Delta)$ and as we can see in fig.4.1 this is confirmed.

4.5.3 The zero-temperature conductivity

Turning our interest towards the conductivity of the 2-site lattice, we need to calculate the current density per link $j_{\frac{1}{2}}(\tau)$ which is

$$\left\langle j_{\frac{1}{2}}(\tau) \right\rangle = -\frac{it}{\hbar}\left(-iG^{<}_{12}(\tau) + iG^{<\dagger}_{12}(\tau)\right) \tag{4.31}$$

according to eq.(C.8) and eq.(4.17). Calculations for the average Fourier transformed current density per link $j_{\frac{1}{2}}(E)$ result in the concise formula

$$\left\langle j_{\frac{1}{2}}(\tau) \right\rangle = \int_{-\infty}^{+\infty} \frac{dE}{2\pi\hbar} \frac{8t^2\hbar^2\Sigma''_L(E)\Sigma''_R(E)\left(N_{\mathrm{FD}}\left(E-(\mu_L-\mu)\right) - N_{\mathrm{FD}}\left(E-(\mu_R-\mu)\right)\right)}{Det\left[G^{+-1}_{aj}(E)\right]^2}, \tag{4.32}$$

which depends on the properties of the reservoirs. Expanding the current to linear order around $\mu_R = \mu$ and $\mu_L = \mu$ results in

$$\left\langle j_{\frac{1}{2}}(\tau) \right\rangle = \int_{-\infty}^{+\infty} \frac{dE}{\pi\hbar} \frac{\left(2t\hbar\Sigma''(E)\right)^2}{Det\left[G^{+-1}_{aj}(E)\right]^2} \frac{\partial N_{FD}(E)}{\partial E}\Delta\mu, \tag{4.33}$$

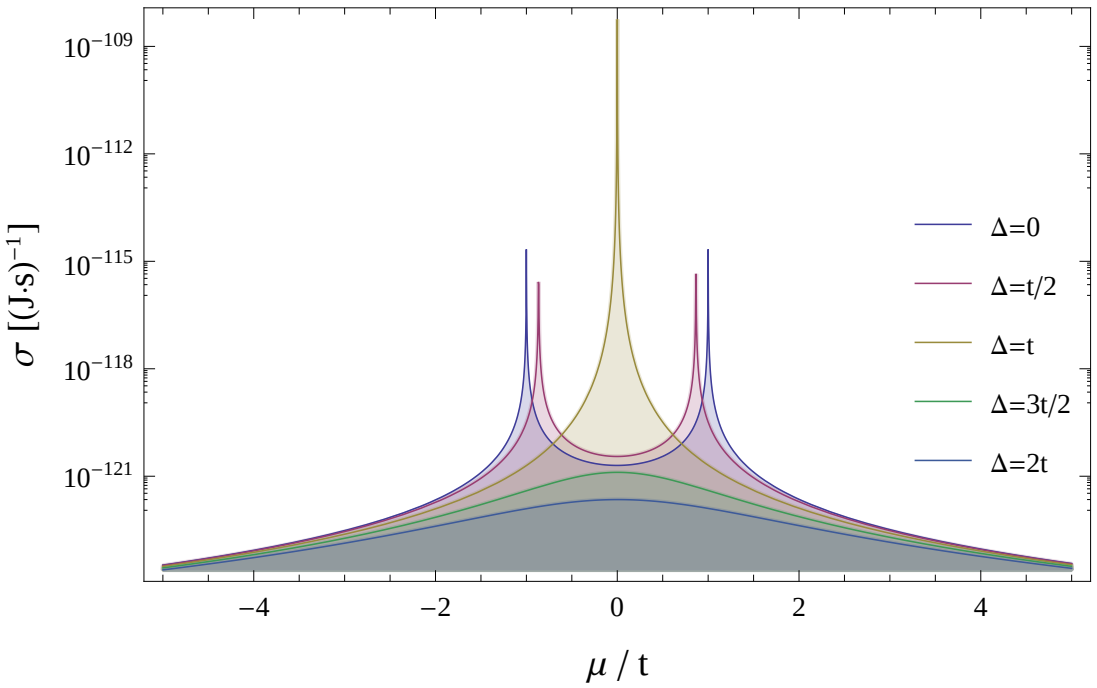

Figure 4.2: The conductivity σ of Kitaev's 2-site lattice at temperature $T = 0$, plotted for $E_{k_0} = -100t$. Maxima are observed at $E = \pm(t \pm \Delta)$, while for $\Delta = t$ which is the phase with Majoranas are present we observe a single maximum which is significantly larger.

where $\Delta\mu = \mu_L - \mu_R$ and $\Sigma_L^{\pm}(E) = \Sigma_R^{\pm}(E) = \Sigma^{\pm}(E)$. Now, the conductivity σ is transparently shown as $\sigma = \frac{\langle j_{1/2}(\tau)\rangle}{\Delta\mu}$ and it is only the integral that needs to be performed in order to get a numerical result.

Taking the zero temperature limit, $T \to 0$, forces the Fermi-Dirac distribution accommodated in the noise correlation function, eq.(4.18), to become a Heaviside $\Theta-$function and its derivative to become a Dirac $\delta-$function peaked at $E = 0$. Subsequently, the integral of eq.(4.33) is easily performed delivering us the current

$$\left\langle j_{\frac{1}{2}}(\tau)\right\rangle\Big|_{T=0} = \frac{2}{h}\frac{\left(2t\hbar\Sigma''(0)\right)^2}{Det\left[G_{aj}^{+-1}(0)\right]^2}\Delta\mu \tag{4.34}$$

and the conductivity

$$\sigma = \frac{2}{h}\frac{4t^2\hbar^2\Sigma''(0)^2}{\left((\mu+\hbar\Sigma'(0))^2+\Delta^2-t^2\right)^2+2\left(\hbar\Sigma''(0)\right)^2\left((\mu+\hbar\Sigma'(0))^2+\Delta^2+t^2\right)+\left(\hbar\Sigma''(0)\right)^4}. \tag{4.35}$$

Plotting the conductivity $\sigma(\mu)$ for several values of Δ, after setting $E_{k_0} = -100t$ gives us fig.4.2 which shows one maximum for $|\Delta| \geqslant t$ and two maxima for $|\Delta| < t$. The maxima always lie within the topological regime of the chemical potential, namely for $|\mu| < 2t$. Of course the phase

where Majorana fermions are present, for the 2-site lattice is expected for $\Delta = t$; there

$$\sigma = \frac{2}{h} \frac{\left(2t\hbar\Sigma''(0)\right)^2}{\left(\left(\mu+\hbar\Sigma'(0)\right)^2+\left(\hbar\Sigma''(0)\right)^2\right)^2+\left(2t\hbar\Sigma''(0)\right)^2} \tag{4.36}$$

and we observe a significantly larger maximum as fig.4.2 clearly shows. According to eq.(4.36) the zero-bias conductivity is $\sigma = 2/h$. Restoring the electron's charge and turning into a frequency $\omega = E/\hbar$ representation for the current $j_{\frac{1}{2}}(\omega)$, see eq.(4.33) results in a zero-bias electrical conductance $G = 2e^2/h$ in agreement with [12]. As a final remark, please note that increasing the superconducting gap Δ in comparison to the hopping amplitude t, so for $\Delta \gg t$, flattens the profile of σ.

Chapter 5

Outlook & Conclusions

Arriving at the end of this thesis I hope the reader has already run into some conclusions but is in parallel at the point of raising questions. First of all, I hope that I have convinced the reader that there is plenty of room for Majorana fermions in condensed matter and that their existence is of great importance thanks to their non-Abelian nature.

According to [13] there are specific requirements for non-Abelian state of matter to occur. Firstly, there must be an energy gap separating the ground state from excited states. This is fulfilled in our model by tuning the hopping amplitude t. As an explicit example, remember that the ground state for the 2-site lattice is separated by the excited ones by $2t$. Secondly, the ground state must be degenerate. This was shown for the general N-site Kitaev model in section 2.4.4. Thirdly, this degeneracy must not be easily lifted by perturbations resulting in a system that - ideally - will not decohere, so it may be used to a build quantum memory (qubit). According to [10] the degeneracy is topologically protected as long as we are within the topological phase ($|\mu| < t$), as explained in section 2.2. Lastly, the exchange of Majoranas, should depend on the quasi-particles trajectory. This makes the system topological and the exchange statistics non-Abelian, since they are dictated by the braiding group instead of the permutations one. May someone here claim that non-Abelian statistics are ill-defined in $1D$ systems and that we need to be in a $2D$ setup, minimally. The answer to this fair concern is the use of T-junctions, networks of $1D$ Kitaev modeled wires, see as it is suggested by [14].

In the second part of the thesis, we investigated the conductivity of Kitaev's model trying to find a signature for the appearance of Majorana fermions. The non-equilibrium methods used proved to be reliable and made us conclude that the maximum of conductivity σ is significantly larger under the presence of Majorana fermions. Our calculation was done for a 2-site lattice and what still remains as a question, but also as a challenge, is to be reproduced for the general case of an N-site lattice. At this point I would like to mention that our result for the conductivity σ is in agrrement to the zero-bias electrical conductance $G = 2e^2/h$ calculated by Karsten Flensberg in [12]. In the case of an N-site lattice, the method is identical but now the Green's functions can no more be treated with "pen & paper" and a the researcher should embark on computer algorithms and numerical techniques.

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The current thesis was part of the Master's programme of Theoretical Physics in "Universiteit Utrecht", aiming to bring the writer in direct contact with current research in Physics. As such I would firstly like to thank my supervisor, Henk T. C. Stoof, for suggesting an "on the edge" topic that proved to be interesting, rich and challenging. But mostly, I would like to thank him for his guidance during all these months, especially for his pedagogical attitude; being always there when I needed him, answering my questions and steering my research towards the "right" direction. I found our discussions always triggering and motivating.

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At this point, I could not forget to pay homage to the distracting steps of the anonymous tall, blonde legs that always made me smile and comforted me during hours of concentration in "Universiteitsbibliotheek Utrecht".

Lastly, I cannot exclude from this "acknowledgements" chapter my family. Their trust and support allowed me to arrive, stay and pursue my ambition to study Theoretical Physics in Utrecht.

Appendix A

The Majorana representation

The usual Pauli matrices are defined as

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{A.1}$$

In Majorana's representation, the γ-matrices of Dirac's equation $(i\gamma^\mu \partial_\mu - m)\,\phi = 0$ are given in terms of the Pauli matrices via

$$\gamma_0 = \sigma_2 \otimes \sigma_1\,, \quad \gamma_1 = i\sigma_1 \otimes \hat{\mathbf{1}}_2, \quad \gamma_2 = i\sigma_3 \otimes \hat{\mathbf{1}}_2, \quad \gamma_3 = i\sigma_2 \otimes \sigma_2 \tag{A.2}$$

Applying the former definition in the latter relations gives

$$\gamma_0 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \gamma_1 = \begin{pmatrix} 0 & 0 & i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix} \gamma_2 = \begin{pmatrix} i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \end{pmatrix} \gamma_3 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{pmatrix} \tag{A.3}$$

showing us the explicit form of the γ-matrices.

Appendix B

Fourier Transforming Kitaev's Hamiltonian

Kitaev's Hamiltonian is by definition given for open boundary conditions since there is one summation up to N_s and another up to N_s-1. Starting with

$$H=-\mu\sum_{i=1}^{N_s}n_i-\sum_{i=1}^{N_s-1}\left[t\left(c_i^\dagger c_{i+1}+c_{i+1}^\dagger c_i\right)-\Delta\left(c_ic_{i+1}+c_{i+1}^\dagger c_i^\dagger\right)\right] \tag{B.1}$$

and inserting $c_i^\dagger=\frac{1}{\sqrt{N_s}}\sum_k e^{-\mathbf{i}k\alpha i}c_k^\dagger$ where $0\leq k\leq\frac{2\pi m}{\alpha N_s}$ and $m=0,1,..,N_s$, gives us

$$\begin{aligned}H=\frac{1}{N_s}\sum_{k,k'}\Bigg\{&-\mu\sum_{i=1}^{N_s}e^{\mathbf{i}(k-k')\alpha i}c_k^\dagger c_{k'}-\sum_{i=1}^{N_s-1}\Big[t\left(e^{\mathbf{i}k\alpha i}e^{-\mathbf{i}k'\alpha(i+1)}c_k^\dagger c_{k'}+e^{\mathbf{i}k\alpha(i+1)}e^{-\mathbf{i}k'\alpha i}c_k^\dagger c_{k'}\right)\\&-\Delta\left(e^{\mathbf{i}\alpha(k'i+k(i+1))}c_{k'}c_k+e^{-\mathbf{i}\alpha(k(i+1)+k'i)}c_k^\dagger c_{k'}^\dagger\right)\Big]\Bigg\}\\=\sum_{k,k'}\Bigg\{&-\mu\left(\frac{1}{N_s}\sum_{i=1}^{N_s}e^{\mathbf{i}(k-k')\alpha i}\right)c_k^\dagger c_{k'}-\frac{N_s-1}{N_s}\frac{1}{N_s-1}\sum_{i=1}^{N_s-1}\Big[te^{\mathbf{i}(k-k')\alpha i}\left(e^{-\mathbf{i}k'\alpha}+e^{\mathbf{i}k\alpha}\right)c_k^\dagger c_{k'}\\&-\Delta\left(e^{\mathbf{i}(k+k')\alpha i}e^{\mathbf{i}k\alpha}c_{k'}c_k+e^{-\mathbf{i}(k+k')\alpha i}e^{-\mathbf{i}k\alpha}c_k^\dagger c_{k'}^\dagger\right)\Big]\Bigg\}\\=\Bigg(&-\mu\sum_{k,k'}c_k^\dagger c_{k'}-t\frac{N_s-1}{N_s}\sum_{k,k'}c_k^\dagger c_{k'}\left(e^{-\mathbf{i}k'\alpha}+e^{\mathbf{i}k\alpha}\right)\Bigg)\delta_{kk'}+\Delta\frac{N_s-1}{N_s}\sum_{k,k'}\left(e^{\mathbf{i}k\alpha}c_{k'}c_k+e^{-\mathbf{i}k\alpha}c_k^\dagger c_{k'}^\dagger\right)\delta_{k,-k'}\end{aligned}$$

resulting in $H=-\sum_k c_k^\dagger c_k\left(\mu+2t\left(1-\frac{1}{N_s}\right)\cos(k\alpha)\right)+\Delta\left(1-\frac{1}{N_s}\right)\sum_k\left(e^{\mathbf{i}k\alpha}c_{-k}c_k+e^{-\mathbf{i}k\alpha}c_k^\dagger c_{-k}^\dagger\right)$.

In case of closed boundary conditions, the Hamiltonian is

$$H=-\mu\sum_{i=1}^{N_s}n_i-\sum_{i=1}^{N_s}\left[t\left(c_i^\dagger c_{i+1}+c_{i+1}^\dagger c_i\right)-\Delta\left(c_ic_{i+1}+c_{i+1}^\dagger c_i^\dagger\right)\right] \tag{B.2}$$

including no different summations up to N_s and N_s-1 within its terms. Fourier transforming

proceeds the same way as before but now the term $\frac{N_s-1}{N_s}$ vanishes resulting in

$$H = -\sum_k c_k^\dagger c_k \left(\mu + 2t\cos\left(k\alpha\right)\right) + \Delta\sum_k \left(e^{\mathbf{i}k\alpha} c_{-k} c_k + e^{-\mathbf{i}k\alpha} c_k^\dagger c_{-k}^\dagger\right). \tag{B.3}$$

Appendix C

The current operator for an $1D$ tight-binding model

Considering the Green's functions for a tight-binding wire given, like the one of eq.(3.30), I am willing to calculate the expectation value for the current field $J(\tau) = \sum_{i=1}^{N_s+1} j_{i-\frac{1}{2}}(\tau)$. The term $j_{i-\frac{1}{2}}(\tau)$ is the current field per link - a point between two sites - defined by satisfying the continuity equation

$$i\frac{dn_i(\tau)}{d\tau} = -\left(j_{i+\frac{1}{2}}(\tau) - j_{i-\frac{1}{2}}(\tau)\right) \tag{C.1}$$

under the boundary conditions $j_{\frac{1}{2}}(\tau) = j_{1+\frac{1}{2}}(\tau)$ and $j_{N_s+\frac{1}{2}}(\tau) = j_{N_s-\frac{1}{2}}(\tau)$. Here τ represents time and we consider $\hbar = 1$.

The fermion density field per site $n_i(\tau)$ is given by the Heisenberg equation

$$\begin{aligned}
\frac{dn_i}{d\tau} &= [H-\mu N, n_i] && \text{(C.2)}\\
&= \left[H-\mu N, \psi_i^\dagger \psi_i\right] \\
&= \psi_i^\dagger \left[H-\mu N, \psi_i\right] + \left[H-\mu N, \psi_i^\dagger\right]\psi_i \\
&= \psi_i^\dagger \left[H-\mu N, \psi_i\right] - \left[H-\mu N, \psi_i\right]^\dagger \psi_i && \text{(C.3)}
\end{aligned}$$

while for Hamiltonians in the form $H-\mu N = \psi_i^\dagger G_{ij}^{-1}\psi_j$ we have $[H-\mu N, \psi_i] = -\sum_{k=1}^{N_s} G_{ik}^{-1}\psi_k$. Combining the above-mentioned gives

$$\begin{aligned}
\frac{dn_i}{d\tau} &= -\psi_i^\dagger\left(\sum_k G_{ik}^{-1}\psi_k\right) + \left(\sum_k G_{ik}^{-1}\psi_k\right)^\dagger \psi_i && \text{(C.4)}\\
&= -2i\,\mathrm{Im}\left[\psi_i^\dagger\left(\sum_k G_{ik}^{-1}\psi_k\right)\right]. && \text{(C.5)}
\end{aligned}$$

This simplifies once we consider the inverse Green's function $G^{-1}_{0;ik}$. In this expression only the nearest-neighboring sites interact, so the current is then given by

$$\begin{aligned}\frac{dn_i}{d\tau} &= -\psi_i^\dagger \left(\cancel{G^{-1}_{0;ii}\psi_i} + G^{-1}_{0;ii+1}\psi_{i+1} + G^{-1}_{0;ii-1}\psi_{i-1}\right) \\ &\quad + \left(\cancel{G^{-1}_{0;ii}\psi_i} + G^{-1}_{0;ii+1}\psi_{i+1} + G^{-1}_{0;ii-1}\psi_{i-1}\right)^\dagger \psi_i \qquad \text{(C.6)} \\ &= t\left(\psi_i^\dagger\psi_{i+1} + \psi_i^\dagger\psi_{i-1} - \psi_{i+1}^\dagger\psi_i - \psi_{i-1}^\dagger\psi_i\right). \qquad \text{(C.7)}\end{aligned}$$

This shows that the current field per link is

$$j_{i\pm\frac{1}{2}}(\tau) = -it\left(\psi_i^\dagger\psi_{i\pm1} - \psi_{i\pm1}^\dagger\psi_i\right) \qquad \text{(C.8)}$$

and consequently the current operator is

$$J(\tau) = -it\sum_{i=1}^{N_s+1}\left(\psi_i^\dagger\psi_{i-1} - \psi_{i-1}^\dagger\psi_i\right). \qquad \text{(C.9)}$$

The electric current is derived when the electron charge e and the lattice spacing R are restored such that

$$J_{el}(\tau) = -|e|RJ(\tau) \qquad \text{(C.10)}$$

while the corresponding electric current density per site is

$$j_{iel}(\tau) = \frac{J_{el}(\tau)}{R} = -|e|J(\tau). \qquad \text{(C.11)}$$

Appendix D

Sokhotski-Plemelj theorem

Theorem. *Sokhotski-Plemelj Theorem: Given a complex-valued function $f(x)$ which is defined and continuous on the real line, while a and b are real constants with $a \leqslant 0 < b$, it holds that*

$$\lim_{\varepsilon \to 0^+} \int_a^b \frac{f(x)}{x \pm i\varepsilon} dx = \mp i\pi f(0)\, dx + \mathcal{P} \int_a^b \frac{f(x)}{x} dx, \tag{D.1}$$

where $\mathcal{P}$ denotes the Cauchy principal value.

In order to apply the theorem for the self-energy of a reservoir, section 4.4.1, we first write eq.4.25 as

$$\Sigma^+(E) = 2m_e t^2 \int_0^{+\infty} \frac{k^2}{k^2 + 2m_e(E - \mu + E_{k_0})} dk = m_e t^2 \int_0^{+\infty} \frac{k}{k^2 + 2m_e(E - \mu + E_{k_0})} d(k^2), \tag{D.2}$$

so if we define $x = k^2$ and $x_0 = 2m_e(E - \mu + E_{k_0})$, we have to apply the theorem on the integral

$$\int_0^{+\infty} \frac{\sqrt{x}}{x + x_0 + i\varepsilon} dx = i\pi\sqrt{x_0} + \mathcal{P} \int_0^{+\infty} \frac{\sqrt{x}}{x - x_0} dx. \tag{D.3}$$

The result is

$$\Sigma^+(E) = m_e t^2 \left(-i\pi \sqrt{2m_e(E - \mu + E_{k_0})} + \mathcal{P} \int_0^{+\infty} \frac{2k^2}{k^2 - 2m_e(E - \mu + E_{k_0})} dk \right) \tag{D.4}$$

which corresponds to eq.4.26.

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