



---

# PHYSICAL PROPERTIES OF SMALL JOSEPHSON JUNCTIONS

BACHELOR'S THESIS

Written by *Waldemar Svejstrup*

June 12, 2019

Supervised by

Brian Møller Andersen

UNIVERSITY OF COPENHAGEN

An abstract geometric design consisting of several overlapping circles and lines, rendered in a light gray color, located in the bottom right corner of the page.



UNIVERSITY OF  
COPENHAGEN

FACULTY: Faculty of Science

INSTITUTE: Niels Bohr Institute

DEPARTMENT: Condensed Matter Theory

AUTHOR: Waldemar Svejstrup

EMAIL: mds274@alumni.ku.dk

TITLE: Physical properties of small Josephson junctions

SUPERVISOR: Brian Møller Andersen

HANDED IN: 12.06.2019

DEFENDED: 21.06.2019

NAME \_\_\_\_\_

SIGNATURE \_\_\_\_\_

DATE \_\_\_\_\_

## **Abstract**

This thesis investigates the physical properties of small Josephson junctions. This is done by first taking basic Josephson junctions into consideration, and through Ginzburg-Landau theory, deriving its characteristics. With the derived characteristics like the current over the junction, circuits containing a Josephson junction are examined. These circuits turn out to have mathematical identical mechanical analogs which are examined as well. Small Josephson junctions under the influence of quantum mechanical effects, are then investigated. The I/V characteristics for small Josephson junctions are found both in the case of a DC-driven model, and in the case of a mixed AC and DC-driven model.

# Contents

|          |  |           |
|----------|--|-----------|
| <b>1</b> | <b>Introduction</b>  | <b>1</b>  |
| <b>2</b> | <b>The physics of Josephson junctions</b>                      | <b>1</b>  |
| 2.1      | Basic Josephson junctions . . . . .                            | 1         |
| 2.2      | Ginzburg-Landau theory . . . . .                               | 2         |
| 2.3      | Current over the junction . . . . .                            | 2         |
| 2.4      | Free energy of the junction . . . . .                          | 3         |
| <b>3</b> | <b>Circuits containing Josephson junctions</b>                 | <b>4</b>  |
| 3.1      | Resistively shunted junction (RSJ) . . . . .                   | 4         |
| 3.2      | Resistively and capacitively shunted junction (RCSJ) . . . . . | 5         |
| 3.2.1    | Overdamped RCSJ . . . . .                                      | 5         |
| <b>4</b> | <b>Mechanical analogs to the RSJ and RCSJ models</b>           | <b>7</b>  |
| 4.1      | The tilted washboard potential . . . . .                       | 8         |
| 4.2      | The mechanical pendulum . . . . .                              | 9         |
| <b>5</b> | <b>Small Josephson junctions</b>                               | <b>9</b>  |
| 5.1      | Commutators and the differentiated bandstructure . . . . .     | 10        |
| 5.2      | The Hamiltonian of small Josephson junctions . . . . .         | 11        |
| 5.3      | Quasicharge . . . . .  | 11        |
| 5.4      | Finding the bandstructure . . . . .                            | 12        |
| 5.5      | Solution to the quasicharge equation . . . . .                 | 14        |
| 5.6      | Small, AC-driven Josephson junctions . . . . .                 | 15        |
| 5.7      | I/V characteristics . . . . .                                  | 16        |
| <b>6</b> | <b>Conclusion</b>  | <b>19</b> |
|          | <b>Appendices</b>  | <b>20</b> |

# 1 Introduction

In 1911, Kamerlingh Onnes discovered that pure mercury lost its electrical resistance abruptly, at some very low critical temperature [1]. This characteristic turned out to apply to several other metals, which formed a completely new branch of physics: Superconductivity. Since Onnes' discovery of superconductivity [2], superconductivity has with its remarkable phenomena continued to amaze scientists up until this very day. After the appearance of satisfactory explanations for superconductivity in the 1950's and 1960's (BCS theory) [2], superconductivity has been further understood. With the understanding of superconductivity, many practical applications have been proposed. In this thesis I investigate the physics of Josephson junctions, which turns out to have practical applications as well. These applications include important topics like SQUIDS, and even proposed applications to quantum bits [3].

This thesis will take its origin in the Ginzburg-Landau theory. Based on this theory, several characteristics of the Josephson junction will be derived, including the free energy, and the current. With the fundamentals of the Josephson junctions derived, I will continue to circuits containing Josephson junctions, and investigate their characteristics. I will show, that these circuits have very close mechanical analogs, which I will investigate. With all these basics of the Josephson junction examined, I move on to an inquiry of small Josephson junctions. For sufficiently small Junctions, quantum mechanical effects have to be taken into account, which complicates the problem, relative to the classical case. In the end, the main goal of this thesis is the I/V characteristics of the Josephson junction, for the cases which I will investigate. I will be looking at a 'big' Josephson junction, i.e. a junction without quantum mechanics, and a both DC and AC-driven small Josephson junction, in which quantum mechanics is taken into account.

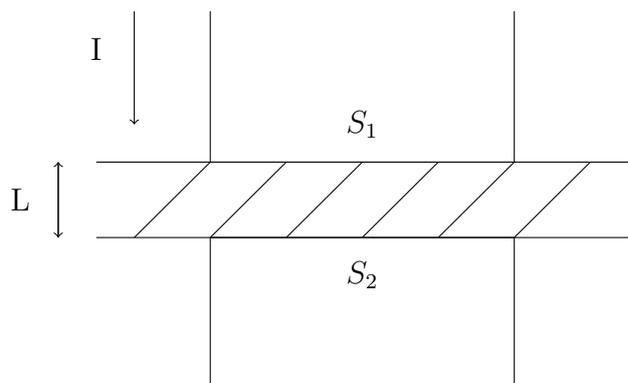
In order to predict the behaviour of an electrical component, one has to know the I/V characteristics. This is therefore essential, for Josephson junctions in practical applications.

## 2 The physics of Josephson junctions

I will start this thesis by considering a basic Josephson junction.

### 2.1 Basic Josephson junctions

A Josephson junction is one superconductor connected to another superconductor, through some non-superconducting material, in this case of length  $L$ . This is schematically shown in figure (1). When one imposes a current across the junction, Josephson effects occur. This is due to the supercurrent led in the two superconductors, being disrupted by the between



**Figure 1:** A simple schematic drawing of a Josephson junction.  $S_1$  and  $S_2$  refers to superconductor 1 and 2.

standing non-superconductive material. The characteristics of this phenomenon is discussed in the following sections [1].

In this thesis, I will define the phase of superconductor 1 and 2 as  $\phi_1$  and  $\phi_2$ , respectively. In the junction however, it is the phase difference between the two superconductors which controls many of the Josephson effects. Therefore I define the difference in phase as [1]:

$$\phi = \phi_1 - \phi_2 \quad (1)$$

## 2.2 Ginzburg-Landau theory

The foundation of this thesis, will be built upon Ginzburg-Landau theory. The Ginzburg-Landau theory assumes that for a small order parameter, the free energy density of a superconductor can be expanded as [2], [4], [5]:

$$f_s = f_n + \alpha|\psi|^2 + \frac{\beta}{2}|\psi|^4 + \frac{1}{2m^*} \left| \left( \frac{\hbar}{i} \nabla + e^* \mathbf{A} \right) \psi \right|^2 + \frac{1}{2\mu_0} (\nabla \times \mathbf{A})^2 \quad (2)$$

Here I will be using the relation  $f = \psi/\psi_\infty$ , where  $\alpha$  and  $\beta$  are parameters defined by  $|\psi_\infty|^2 = -\frac{\alpha}{\beta}$  [2].  $\psi$  is the collective wavefunction of the electrons (or more precisely Cooper pairs which is why we have effective mass and charge). Apart from that, we have the normal state energy,  $f_n$ , the vector potential  $\mathbf{A}$ , the effective mass  $m^*$ , and the effective charge  $e^*$ . Please note that  $\psi_\infty$  is defined such that, when the material described is in equilibrium,  $|f| = 1$ .

Another Ginzburg-Landau equation I will be using in this thesis, is the Ginzburg-Landau current expression [2], [4]:

$$\mathbf{J} = \frac{e^* \hbar}{2m^* i} (\psi^* \nabla \psi - \psi \nabla \psi^*) - \frac{e^{*2}}{m^*} \psi^* \psi \mathbf{A} \quad (3)$$

This equation is often referred to as the second Ginzburg-Landau equation [4], and gives an expression for the current density,  $\mathbf{J}$ . It can be obtained by minimizing equation (2) with respect to  $\mathbf{A}$ , and invoking Maxwell's 4th equation (Ampère's law) [4]. Later on, I will assume the current to move only in the x-direction, and thus write the current as a scalar instead of a vector. The two equations, (2) and (3), are very powerful and will form the foundation of this thesis.

## 2.3 Current over the junction

To describe the current over a simple Josephson junction, we start off by looking at equation (2). We will describe the simplest possible case, and thus we remove the vector potential:  $\mathbf{A} = \bar{0}$ . The wavefunction will try to minimize the free energy, and by doing the functional derivatives with respect to  $\psi$  and  $\psi^*$  [4] one reaches, what is often referred to as the first Ginzburg-Landau equation [2]:

$$\frac{\hbar^2}{2m^*} \nabla^2 \psi + \alpha \psi + \beta |\psi|^2 \psi = 0 \quad (4)$$

Assuming only spatial dependence of the wavefunction in the x-direction, recalling that  $|\psi_\infty|^2 = -\alpha/\beta$ , defining the coherence length as  $\xi = \hbar/\sqrt{|2m^*\alpha|}$ , and rewriting  $\psi$  as  $f$  through the relation  $f = \psi/\psi_\infty$  we get [2]:

$$\xi^2 \frac{d^2 f}{dx^2} + f - f^3 = 0 \quad (5)$$

We can describe  $f$  in the following way,  $f = e^{i\phi}$ , and thus in the limit where the length of the bridge  $L$  is much smaller than the coherence length:  $L \ll \xi$ , the first term in equation (5) will dominate the two other terms. This is because we can choose  $\xi$  to be arbitrarily much larger than  $L$ , and thus the term including  $\xi^2$  will become much larger than the others. For a more detailed discussion of this, one can see reference [2]. Thus we can approximate equation (5) to:

$$\frac{d^2 f}{dx^2} = 0 \quad (6)$$

If we set the start of the bridge at  $x = 0$ , and the end of it in  $x = L$ , we get the boundary conditions,  $f = 1$  at  $x = 0$ , and  $f = e^{i\phi}$  at  $x = L$ . Thus, the equation for  $f$  must be [2]:

$$f = 1 - \frac{x}{L} + \frac{x}{L} e^{i\phi} \quad (7)$$

If we insert this expression for  $f$  into the Ginzburg-Landau current expression (equation (3)), setting  $\mathbf{A} = \bar{0}$ , we get [2]:

$$J = \frac{e^* \hbar}{2m^* i} (\psi^* \nabla \psi - \psi \nabla \psi^*) \quad (8)$$

Realising that  $\nabla = \frac{d}{dx}$ , because we assume our order parameter only to have spatial dependence in the x-direction, we get that:

$$J = \psi_\infty^2 \frac{e^* \hbar}{m^* L} \sin(\phi) \quad (9)$$

Since  $J$  is the current density, we get that the current  $I$ , must be equal to the cross section area of the junction, times the current density. Thus we get that:

$$I = JA = \psi_\infty^2 \frac{2e^* \hbar A}{m^* L} \sin(\phi) = I_{c0} \sin(\phi) \quad (10)$$

Where we remember that  $e^* = 2e$  and have defined  $I_{c0} = \frac{\psi_\infty^2 2e^* \hbar A}{m^* L}$  [2]. This means, that the current through the junction oscillates between  $-I_{c0}$  and  $I_{c0}$ , with a periodic phase of  $\pi$ . The current  $I_{c0}$  is called the Josephson critical current.

## 2.4 Free energy of the junction

Starting from the Ginzburg-Landau equation (2), but now defining  $f_n = 0$ ,  $\mathbf{A} = \bar{0}$ , we get the free energy density:

$$f_s = \alpha |\psi|^2 + \frac{\beta}{2} |\psi|^4 + \frac{1}{2m^*} \left| \frac{\hbar}{i} \nabla \psi \right|^2 \quad (11)$$

But using the wavefunction  $f = \psi/\psi_\infty$ , and the relation  $|\psi_\infty|^2 = -\frac{\alpha}{\beta}$  [2], we get the relation for the free energy density:

$$f_s = \alpha |\psi|^2 - \frac{\alpha}{2} |f|^2 |\psi|^2 + \frac{1}{2m^*} \left| \frac{\hbar}{i} \nabla \psi \right|^2 \quad (12)$$

In order to get the free energy of the junction, one has to integrate over the entire junction. In our case, we are considering a 3-D junction, and must therefore take all

three directions into consideration. If we assume, that the energy density only has spatial dependence in the direction of the current (in our case, the x-direction), we get the following expression for the free energy,  $\Delta F$

$$\Delta F = \int_0^{L_y} \int_0^{L_z} \int_0^L f_s dx dz dy = A \int_0^L f_s dx \quad (13)$$

Where  $L$  is the length of the junction in the x-direction, and  $A$  is the cross sectional area. Please note, that one could argue, that the free energy on both sides of the junction, is affected by the junctions influence on the order parameter. Furthermore, one could argue, that the free energy has to be somewhat different, at least one coherence length both before, and after the junction itself. However, we are only interested in the free energy in the junction itself, and will thus only integrate from 0 to  $L$ , in the direction of the current. When we do the integration for the free energy, we get:

$$\Delta F = -A \frac{\alpha}{2} |\psi_\infty|^2 (-L + \frac{8}{15} L \sin^4(\phi/2)) + \frac{\hbar}{2e} I_{c0} (1 - \cos(\phi)) \quad (14)$$

Here we have used  $I_{c0} = \frac{2e\hbar\psi_\infty^2 A}{m^*L}$ . By using the relation  $\xi = \hbar/\sqrt{|2m^*\alpha|}$  [2], we can rewrite the first part of the free energy to contain  $\frac{L}{\xi^2}$  [2], which goes to zero with  $L \ll \xi$ . Therefore we get the free energy [2]:

$$\Delta F = \frac{\hbar}{2e} I_{c0} (1 - \cos(\phi)) = E_J (1 - \cos(\phi)) \quad (15)$$

Where, in the last equation, I have defined  $E_J = \frac{\hbar}{2e} I_{c0}$ . This turns out to be an important result, because the phase dependent part,  $E_J \cos(\phi)$ , will serve as the potential in our Hamiltonian later on.

### 3 Circuits containing Josephson junctions

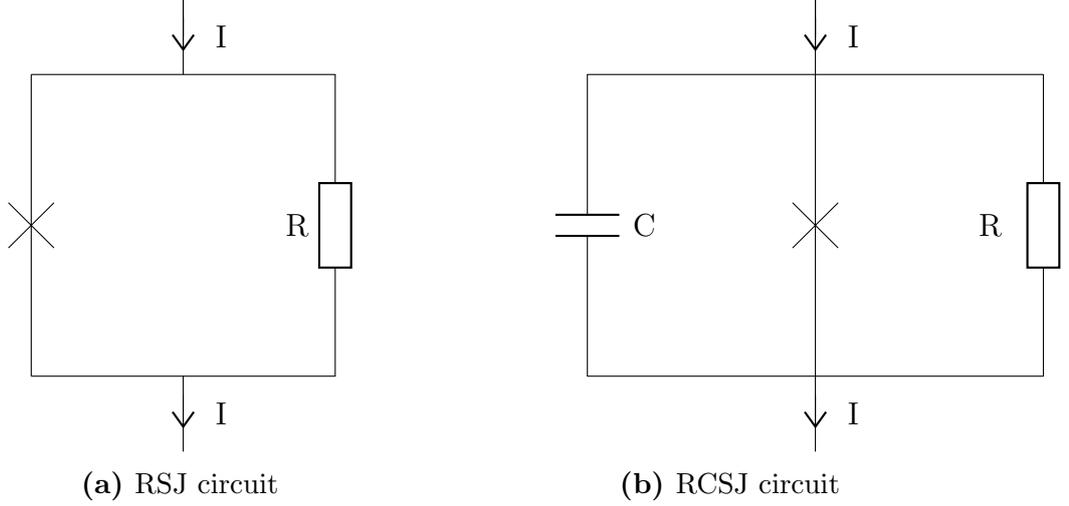
We will be considering two general circuits, involving Josephson junctions. The two models are the RSJ (resistively shunted junction) model, and the RCSJ (resistively and capacitively shunted junction). See figure (2a) and (2b) respectively.

#### 3.1 Resistively shunted junction (RSJ)

The first system we are going to examine is the so called RSJ model. This model is simply a Josephson junction and a resistor, put in parallel circuit with each other. For a schematic drawing, see figure (2a). We now imagine, driving the Josephson effects, by imposing some current,  $I$ , over the circuit. By using equation (10), we see that the current going through the entire circuit must be [1]:

$$I = I_{c0} \sin(\phi) + \frac{V}{R} \quad (16)$$

Where  $V/R$  simply comes from Ohm's law. Before we solve this, we are going to define some constants, and use some relations, which is showed on the RCSJ model. However, we will come back to this problem, when discussing the overdamped RCSJ, which is essentially the RCSJ model, approximated to be like the RSJ model [1]. More precisely, we are going to examine the more general RCSJ model, and then interpret the RSJ model, as a simplified case with very small capacitance.



**Figure 2:** The two circuits we will consider. The Josephson junction is marked with a cross.

### 3.2 Resistively and capacitively shunted junction (RCSJ)

We will now consider a circuit, containing both a Josephson junction, some resistance,  $R$ , and some capacitance,  $C$ , all connected in parallel. This can be seen in figure (2b). One would get that the current running through the system must be [2]:

$$I = I_{c0} \sin(\phi) + \frac{V}{R} + C \frac{dV}{dt} \quad (17)$$

Where  $\phi$  is the phase difference across the junction,  $V$  is the voltage across the system, and  $t$  is simply time. By using the relation [2]:

$$\frac{d\phi}{dt} = \frac{2eV}{\hbar} \quad (18)$$

We can write equation (17) as:

$$I = I_{c0} \sin(\phi) + \frac{\hbar}{2eR} \frac{d\phi}{dt} + C \frac{d}{dt} \left( \frac{\hbar}{2e} \frac{d\phi}{dt} \right) = I_{c0} \sin(\phi) + \frac{\hbar}{2eR} \frac{d\phi}{dt} + \frac{C\hbar}{2e} \frac{d^2\phi}{dt^2} \quad (19)$$

If we introduce the new parameters [2]:

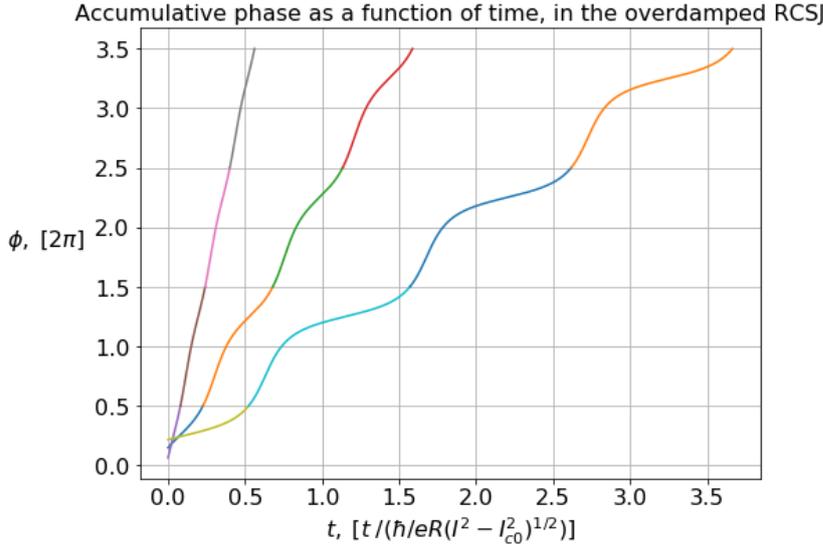
$$\tau = \omega_p t, \quad \omega_p = \left( \frac{2eI_{c0}}{\hbar C} \right)^{1/2}, \quad Q = \omega_p RC \quad (20)$$

And divide by  $I_{c0}$ , we get the new differential equation, describing the current through the circuit [2]:

$$\frac{I}{I_{c0}} = \sin(\phi) + \frac{1}{Q} \frac{d\phi}{d\tau} + \frac{d^2\phi}{d\tau^2} \quad (21)$$

#### 3.2.1 Overdamped RCSJ

In what we describe as an overdamped junction, we have a very small capacitance,  $C$ . From equation (20), we get that  $C$  goes as  $Q^2$ . Thus we get that in an overdamped junction,  $Q \ll 1$ . Therefore we can write equation (21) as:



**Figure 3:** Phase as a function of time, for 3 different values of  $I/I_{c0}$ . Every time the phase increases by  $2\pi$ , the graph changes color. The flattest graph:  $I/I_{c0} = 1.25$ , The middle graph:  $I/I_{c0} = 2$ , The steepest graph:  $I/I_{c0} = 5$

$$\frac{I}{I_{c0}} = \sin(\phi) + \frac{1}{Q} \frac{d\phi}{d\tau} \quad (22)$$

This can also be written in terms of  $t$ , as [2]:

$$\frac{d\phi}{dt} = \frac{2eI_{c0}R}{\hbar} \left( \frac{I}{I_{c0}} - \sin(\phi) \right) \quad (23)$$

This has the solution for the phase difference:

$$\phi = 2 \arctan \left( \frac{\tan \left( \frac{eR\sqrt{I^2 - I_{c0}^2}}{\hbar} (t + k) \right) \sqrt{I^2 - I_{c0}^2} + I_{c0}}{I} \right), \quad (24)$$

where  $k$  is a constant of integration. However, since  $k$  is just added to the time  $t$ , this is physically just a constant of time. By deciding when we start the time, I can simply put  $k = 0$ . The phase is plotted in figure (3). One should be aware, that I have plotted the entire phase difference, and not just the net phase difference, thus I call it an 'accumulative' phase on the plot. The current through the circuit, is however only interested in the 'net' phase difference, since for instance  $\cos(3\pi) = \cos(\pi)$ . Since the only time dependence of the phase in equation (24) is in the tan expression, we can easily extract the period of the phase. We see, that since tan is periodic in integers of  $\pi$ , the period must be given by

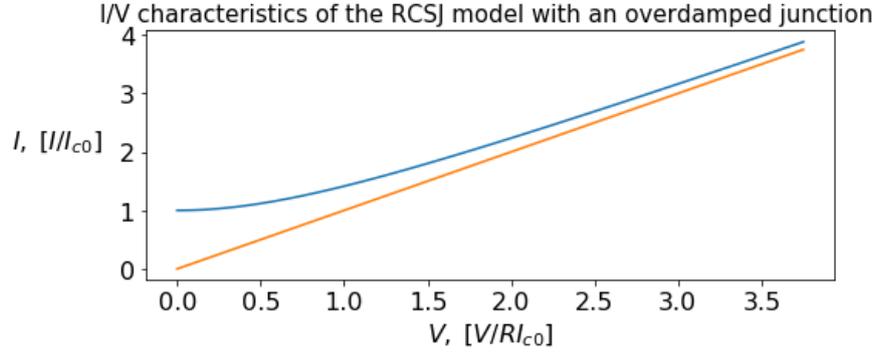
$$T = \frac{\pi\hbar}{eR\sqrt{I^2 - I_{c0}^2}} \quad (25)$$

We then seek to find the average voltage over a period of time,  $T$ . Since  $\phi$  is periodic in exactly this time interval, we get that  $\phi$  must increase by  $\pi$ , when time increases with  $T$ . We see that the voltage must be given by equation (18), and that we can easily average over a time period,  $T$ .

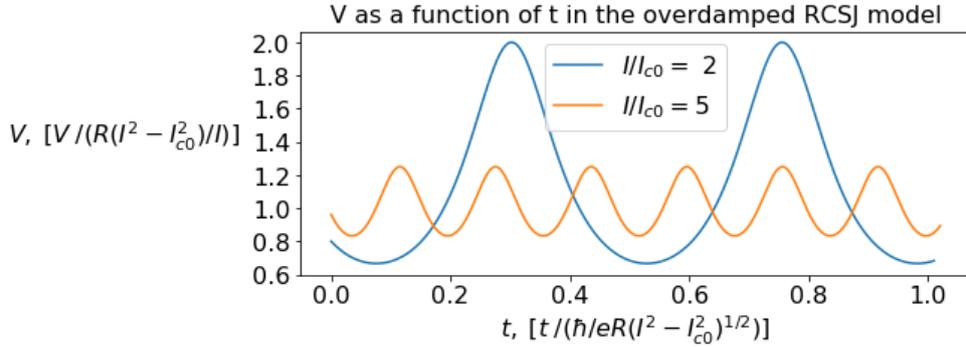
$$\bar{V} = \frac{\hbar}{2e} \frac{d\bar{\phi}}{dt} = \frac{\hbar}{2e} \frac{2\pi}{T} = \frac{\hbar}{2e} \frac{2\pi eR\sqrt{I^2 - I_{c0}^2}}{\pi\hbar} = R\sqrt{I^2 - I_{c0}^2} \quad (26)$$

Where  $\bar{V}$  and  $\frac{\bar{d\phi}}{dt}$  refer to the average voltage and the average change of phase, respectively. The average voltage gives rise to the I/V characteristics that can be seen in figure (4). One sees that when the current is equal to  $I_{c0}$ , we have no voltage across the system. In this regime, we have a supercurrent running in the circuit. However, at higher currents, the voltage increases, and the I/V characteristics approaches the usual ohmic behaviour.

Instead of averaging over time, we could also take the expression for the phase, that we find in equation (24), and use the relation between the voltage and differentiated phase, found in equation (18), to obtain an expression for the voltage, as a function of time [6]. This can be seen in figure (5).



**Figure 4:** Time averaged I/V characteristics, for the overdamped RCSJ model. Blue graph is the voltage given in equation (26), orange graph is the simple ohmic relation,  $V = RI$



**Figure 5:** Voltage as a function of time in the overdamped RCSJ model, for two different values of  $I/I_{c0}$

## 4 Mechanical analogs to the RSJ and RCSJ models

Physical parallels can be drawn from both the RSJ and RCSJ models. These illustrate the principles, and the math behind the phenomena.

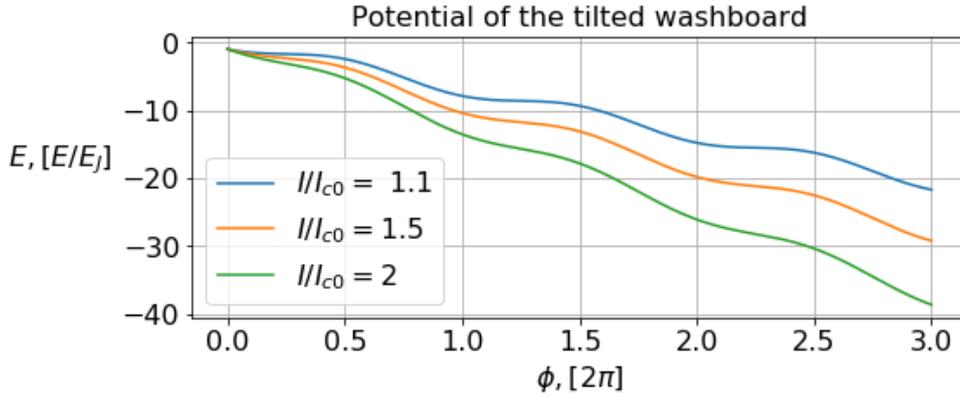
## 4.1 The tilted washboard potential

We are first to consider a particle on a tilted washboard-like potential, which can be seen in figure (6). We then imagine the particle being influenced by a gravity-like force, pointing downwards, and some form of sticky substance, giving the particle a drag force opposite to its direction of motion. We are going to mathematically describe the tilted washboard potential, and the sticky drag force respectively:

$$U(x) = -E_J \cos(x) - \frac{\hbar I}{2e} x, \quad F_{drag} = \left(\frac{\hbar}{2e}\right)^2 \frac{1}{R} \dot{x} \quad (27)$$

Here  $x$  is the distance travelled down the potential by the particle, and  $\dot{x}$  is the derivative of  $x$  with respect to time, which of course is the particles velocity. Using Newton's second law we obtain:

$$m\ddot{x} = -\frac{\partial}{\partial x}U(x) - \left(\frac{\hbar}{2e}\right)^2 \frac{1}{R} \dot{x} \quad (28)$$



**Figure 6:** Potential of the tilted washboard for 3 different values of  $I/I_{c0}$

Now defining the following relations [2]:

$$m = \left(\frac{\hbar}{2e}\right)^2 C, \quad E_j = \frac{\hbar}{2e} I_{c0}, \quad Q = \omega_p RC, \quad \omega_p = \sqrt{\frac{2eI_{c0}}{\hbar C}} \quad (29)$$

We can rewrite equation (28) as:

$$\omega_p^{-2} \ddot{x} + \omega_p \frac{1}{CR} \dot{x} + \sin(x) = \frac{I}{I_{c0}} \quad (30)$$

If we now change the variable from  $t$  to  $\tau$ , remembering that  $\tau = \omega_p t$  we get that:

$$\dot{x} = \frac{\partial}{\partial t} x = \omega_p \frac{\partial}{\partial \tau} x \quad (31)$$

And we can thus write equation (30) as:

$$\frac{\partial^2}{\partial \tau^2} x + \frac{1}{Q} \frac{\partial}{\partial \tau} x + \sin(x) = \frac{I}{I_{c0}} \quad (32)$$

But, replacing the  $x$  with  $\phi$ , we see that equation (32) is exactly identical to equation (21). Therefore we see, that solving the RCSJ model, is exactly the same as solving the equation of motion, for a particle on a tilted washboard, with a sticky drag. One can simply interpret the phase, as the distance covered by the particle, along the potential. If one were to remove the sticky drag from the potential, we would remove the double differentiated term of equation (32), and would therefore get:

$$\frac{1}{Q} \frac{\partial}{\partial \tau} x + \sin(x) = \frac{I}{I_{c0}} \quad (33)$$

Which again, when  $x$  is substituted with  $\phi$ , is exactly the same as equation (22). Thus solving the RSJ model (or overdamped RCSJ), is exactly the same as solving the equation of motion for a particle sliding down a tilted washboard.

## 4.2 The mechanical pendulum

Another physical parallel is a simple pendulum with an applied torque. We imagine a pendulum of weight  $m$ , hanging a distance  $l$  from an axis it can rotate around. The pendulum is attached to a weight of mass  $m_w$ , which performs a torque on the pendulum due to a displacement of length  $r$ , to the axis which the pendulum rotates about. See figure (7b) for a schematic of the pendulum [6]. The pendulum is in total affected by 3 different torques. A torque due to the added weight, which is given by  $\tau_a = m_w r g$ , where  $g$  is the gravitational acceleration. A torque due to gravity on the pendulum itself, given by  $\tau_g = -mgl \sin(\theta)$ . A torque due to friction in the system,  $\tau_f = -D_f \frac{d\theta}{dt}$ , where  $D_f$  is a damping coefficient. The sum of these 3 torques must be equal to the total moment of inertia of the system,  $M_I$ , times the angle,  $\theta$  differentiated twice with respect to time:

$$M_I \frac{d^2\theta}{dt^2} = m_w r g - mgl \sin(\theta) - D_f \frac{d\theta}{dt} \quad (34)$$

If we consider the applied torque  $\tau_a = m_w r g$  as a constant, we can write the equation:

$$\tau_a = M_I \frac{d^2\theta}{dt^2} + D_f \frac{d\theta}{dt} + mgl \sin(\theta) \quad (35)$$

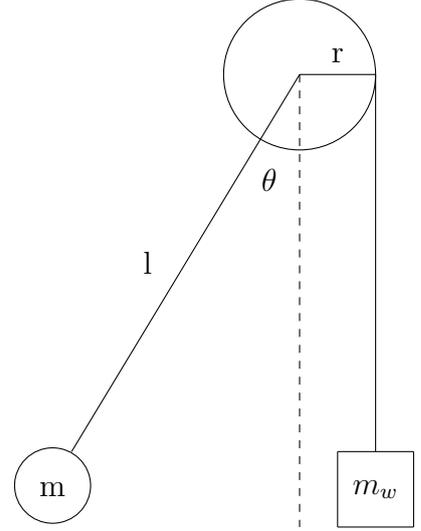
Which is analogous to equation (19). We can thus conclude, that the RCSJ model is mathematically identical to the mechanical pendulum [6]. We quickly see by comparison of equation (19) and (35), that all the electrical quantities, has direct mechanical analogs. These analogs can be seen in figure (7a).

## 5 Small Josephson junctions

So far we have been describing systems with large Josephson junctions. When describing such 'large' systems, one does not have to take quantum mechanics into consideration. In our case however, we will try to describe a Josephson junction so small, that we have to take quantum mechanics into account. Our starting point will be a Hamiltonian, from where we will calculate the bandstructure of the system, equations for the quasicharge, and in the end, the I/V characteristics. In order to do this, we will need some general results from condensed matter physics.

| Electrical quantity        | Mechanical analog                |
|----------------------------|----------------------------------|
| Total current, $I$         | Applied torque, $\tau_a$         |
| Critical current, $I_{c0}$ | Torque due to gravity, $mgl$     |
| Conductance, $1/R$         | Damping, $D_f$                   |
| Capacitance, $C$           | Moment of inertia, $M_I$         |
| Phase difference, $\phi$   | Angle from equilibrium, $\theta$ |

(a) Electrical quantities and their mechanical analogs



(b) Pendulum with applied torque

**Figure 7:** Table of our electrical quantities with their mechanical analogs, and a schematic drawing of the mechanical pendulum

## 5.1 Commutators and the differentiated bandstructure

We will take a look at the very general result from superconductivity physics, namely that phase,  $\phi$ , and number of electrons,  $N$  (ordered in cooper pairs), does not commute:  $[\phi, N] \neq 0$ . Thus, if the number of electrons is completely determined, then the phase must be completely undetermined. If the phase is completely undetermined, then there will be no supercurrent running in the superconductor. This goes the other way around as well: If you have the phase completely determined, then the number of electrons must be completely undetermined, and thus you can have a supercurrent in the superconductor. This relation turns out to concern the phase, and the quasicharge as well, in the following way:

$$[\phi, q] = 2ei \quad (36)$$

Because we can only have superconductivity with a well-defined phase, we realise, that for superconductivity to take place, we must have an undefined quasicharge. This commutator relation will turn out to be essential, not only in the calculations below, but also in the interpretation of the  $I/V$  curves in the end.

Another important relation I will be using in the calculations below, will be:

$$V = \frac{dE^{(0)}}{dq} \quad (37)$$

This means, that I will describe the slope of the lowest bandstructure in  $q$ -space, as the voltage across the junction. Below I will, to some extent, justify this relation, but for a rigorous proof, one should see reference [7].

Since we know that the lattice (and thus also the potential) is periodic and obeys both differentiability and continuity at all times, one could approximate the bandstructure, to a sum of parabolas. Firstly, we will assume that the lowest bandstructure, call it  $H_0$ , is on the parabolic form,  $H_0 = E_0 q^2$ , where  $E_0$  is some constant, and  $q$  is the quasicharge. We could then use the commutation relation in the Heisenberg picture,

in order to get an expression for the differentiated phase,  $\dot{\phi}$ . The commutation relation [8] [9] in the Heisenberg picture states that:

$$\dot{A} = \frac{1}{i\hbar}[A, H] \quad (38)$$

Where  $A$  is some operator, and  $H$  is the Hamiltonian. We would thus get that:

$$\begin{aligned} \dot{\phi} &= \frac{1}{i\hbar}[\phi, H_0] = \frac{1}{i\hbar}[\phi, E_0q^2] = \frac{E_0}{i\hbar}[\phi, qq] \\ &= \frac{E_0}{i\hbar}(-q[q, \phi] - [q, \phi]q) = \frac{E_0}{i\hbar}(q2ei + 2eiq) = \frac{E_0}{i\hbar}(4qei) = \frac{4E_0qe}{\hbar} \end{aligned} \quad (39)$$

Here we can use equation (18), and thus get:

$$\dot{\phi} = \frac{2e}{\hbar}V = \frac{4E_0qe}{\hbar} \rightarrow V = 2E_0q \quad (40)$$

We now realise, that  $\frac{dH_0}{dq} = 2E_0q$ , and we can therefore, in our example, conclude that the voltage is indeed, equal to the derivative of the lowest bandstructure. Later we will see plots of the lowest bandstructure (figure 9), which indeed seems to have the shape of parabolas.

## 5.2 The Hamiltonian of small Josephson junctions

We will be considering a Hamiltonian, which has no coupling to the junction environment, but which does take quantum mechanical effects into account. Such a Hamiltonian [7], is described by:

$$H = \frac{Q^2}{2C} + U(\phi) - \frac{\hbar}{2e}I(t)\phi + \frac{\hbar}{2e}I_q(x)\phi \quad (41)$$

Where  $Q$  is the charge,  $C$  is the capacitance,  $U(\phi)$  is the potential as a function of phase difference,  $I(t)$  is the current, and  $I_q(x)$  is the quasiparticle current. Using the relations [7]:

$$Q = \frac{2e}{i} \frac{\partial}{\partial \phi} \quad E_Q = \frac{e^2}{2C} \quad U(\phi) = E_J \cos(\phi) \quad (42)$$

The first relation comes from equation (36) and the fact that the commutator must stay the same if we exchange  $q$  with the total charge,  $Q$ . We can thus describe our Hamiltonian in equation (41) as:

$$H = - \left( E_Q \frac{\partial^2}{\partial(\phi/2)^2} + E_J \cos(\phi) \right) - \frac{\hbar}{2e}I(t)\phi + \frac{\hbar}{2e}I_q(x)\phi \quad (43)$$

With this Hamiltonian, we are ready to begin our description of the quasicharge.

## 5.3 Quasicharge

We start our examination of the quasicharge, by using the commutation relation in the Heisenberg picture. We will assume, that the only parts of the Hamiltonian in equation (43), that has a non-zero commutator with  $q$ , are the last two terms (i.e. the terms including  $I(t)$  and  $I_q(x)$ ). For a more detailed discussion of this, one can see

reference [7].

From the Heisenberg picture, we can obtain an equation for the differentiated quasicharge:

$$\dot{q} = \frac{1}{i\hbar}[q, H] = \frac{1}{i\hbar}\left[q, -\frac{\hbar}{2e}I(t)\phi + \frac{\hbar}{2e}I_q(x)\phi\right] = \frac{1}{2ei}\left(-[q, I(t)\phi] + [q, I_q(x)\phi]\right) \quad (44)$$

By realizing that neither of the current expressions ( $I(t)$  and  $I_q(x)$ ) has phase dependence, and using the relation in equation (36), we can rewrite equation (44) as:

$$\dot{q} = \frac{1}{2ei}\left(-I(t)[q, \phi] + I_q(x)[q, \phi]\right) = \frac{1}{2ei}\left(I(t)2ei - I_q(x)2ei\right) = I(t) - I_q(x) \quad (45)$$

Under the assumption that the junction is completely isolated from the environment (which we assumed when writing our Hamiltonian), the quasiparticle current can be expressed [7] as:

$$I_q(x) = GV \quad (46)$$

Where  $V$  is the voltage, and  $G$  is the quasiparticle conductivity [7]. This means that we can now express the differential equation for the quasicharge from equation (45) as:

$$\dot{q} = I(t) - GV \quad (47)$$

At this point, we will use the fact that the voltage is just the quasicharge-derivative of the lowest bandstructure, as shown in equation (37). We can thus replace the voltage in equation (47) to obtain:

$$\dot{q} = I(t) - G\frac{dE^{(0)}}{dq} \quad (48)$$

In order to solve this differential equation for the quasicharge, we are going to use straightforward integration. First we will assume to have a direct current, which causes  $I(t)$  to have no time dependence, and we will thus call it  $I$ . We then reach the following equation:

$$\int \frac{dq}{dt} dt = q(t) = \int I - G\frac{dE^{(0)}}{dq} dt \quad (49)$$

In order to solve this, one must have some function or numerical values for the lowest band in the band structure,  $E^{(0)}$ .

## 5.4 Finding the bandstructure

In our quest for finding the bandstructure, we will first consider the potential of the Hamiltonian in equation (43):

$$U(\phi) = E_J \cos(\phi) \quad (50)$$

Realising that the crystal lattice is periodic with a lattice constant which I will define as  $a$ , and using that our potential is periodic in  $2\pi$ , I can write the potential as [10]:

$$U(x) = E_J \cos\left(\frac{2\pi}{a}x\right), \quad (51)$$

where I define  $x$  to be distance along the lattice. We now realize, that this of course can be written as a sum of two exponentials:

$$U(x) = \frac{E_J}{2} \left( e^{i\frac{2\pi}{a}x} + e^{-i\frac{2\pi}{a}x} \right) \quad (52)$$

We will now define the reciprocal lattice vector,  $G$ , and we quickly see that because  $e^{iGR} = 1$ , where  $R$  is the lattice position vector, must be true, we must have that  $G_n = \frac{2\pi}{a}n$ , where  $n$  is some integer. Please note that both  $G$  and  $R$  are vectors. However since we are considering only one dimension of spatial variables, both  $G$  and  $R$  are treated as simple scalars. After this conclusion, we can define  $G_1 = \frac{2\pi}{a}$  and write our potential as:

$$U(x) = \frac{E_J}{2} \left( e^{iG_1x} + e^{-iG_1x} \right) \quad (53)$$

From here, we will use a result from reference [10]. This result is known as the central equation, which will not be proved in this thesis. The central equations is as follows:

$$(\lambda_k - E_k)C(k) + \sum_G U_G C(k - G) = 0, \quad \lambda_k = \frac{\hbar^2 k^2}{2m} \quad (54)$$

Where  $C(k)$  is some  $k$ -dependent constant to the wavefunction, and  $k$  is the wavevector (again, treated as a scalar).  $U_G$  is the constant in front of our exponential functions, in our potential, i.e.  $U_G = E_J/2$ , and  $E_k$  is the bandstructure, for a given  $k$  (one should keep in mind, that  $E_J$  is still just a constant energy, and not a part of the bandstructure,  $E_k$ ). We can thus insert our potential in equation (54), but can do this for any value of  $k$ . As a start, we could just choose some arbitrary  $k$ :

$$(\lambda_k - E_k)C(k) + \frac{E_J}{2}C(k - G_1) + \frac{E_J}{2}C(k + G_1) \quad (55)$$

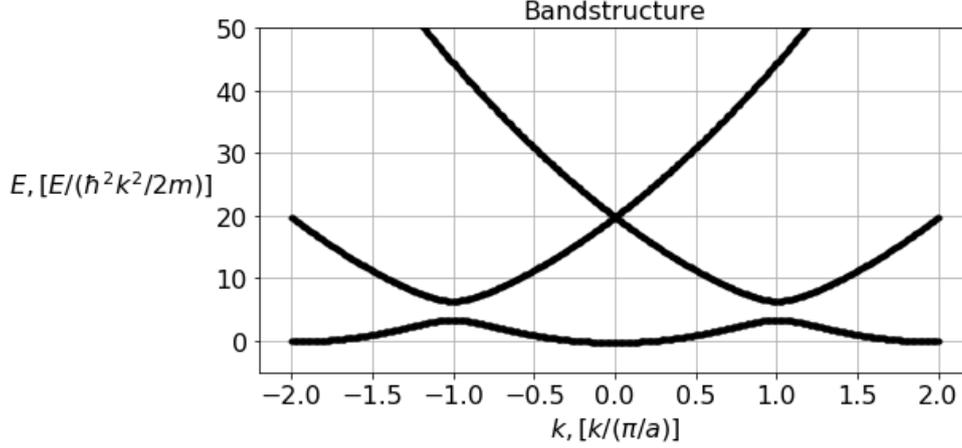
However, we could also do the same for,  $k - G_1$  or  $k + G_1$ . If we were to write the same equation, but for  $k - G_1$ , we would get:

$$(\lambda_{k-G_1} - E_{k-G_1})C(k - G_1) + \frac{E_J}{2}C(k - 2G_1) + \frac{E_J}{2}C(k) \quad (56)$$

Continuing this way, one can construct as many equations as one wants, describing the bandstructure. Say, that one starts of by writing an equation, starting with  $k$ , and then continues to write  $n$  equations below  $k$ . This would mean all equations containing  $\lambda_k, \lambda_{k-G}, \lambda_{k-2G}, \dots, \lambda_{k-nG}$ . Correspondingly, one could write  $n$  equations above  $k$ , in the same way. Thus, one would get  $n+n+1 = 2n+1$  coupled equations, all describing the bandstructure. We are however, when doing this, going to approximate any terms containing higher orders of  $G$  than  $n$ , to zero [10]. This means, that we can write all our equations in the following way:

$$\begin{bmatrix} (\lambda_{k-G} - E_{k-G}) & \frac{E_J}{2} & 0 \\ \frac{E_J}{2} & (\lambda_k - E_k) & \frac{E_J}{2} \\ 0 & \frac{E_J}{2} & (\lambda_{k+G} - E_{k+G}) \end{bmatrix} \cdot \begin{bmatrix} C_{k-G} \\ C_k \\ C_{k+G} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad (57)$$

Equation (57) is shown with 3 equations (i.e.  $n = 3$ ), but could be generalized to any size. This equation makes the quest for the bandstructure,  $E_k$ , an eigenvalue problem. This can be solved numerically, and gives a bandstructure as can be seen in figure (8)



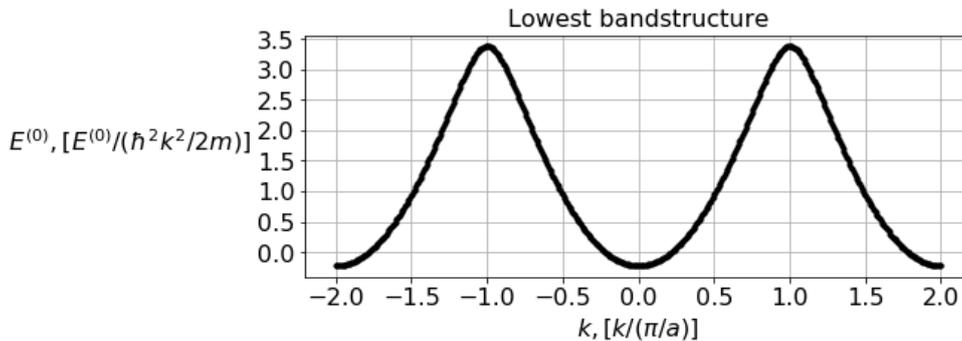
**Figure 8:** Bandstructure for our Hamiltonian. Here plotted with  $n = 3$ , and  $E_J = 3\frac{\hbar^2 k^2}{2m}$

Here I will define the lowest bandstructure as  $E^{(0)}$ , which is the term that I have already previously used. In the appendix, one can find a python script, which among other things, numerically calculates the bandstructure, for  $n = 11$ . This value for  $n$  can be set to any positive, uneven integer.

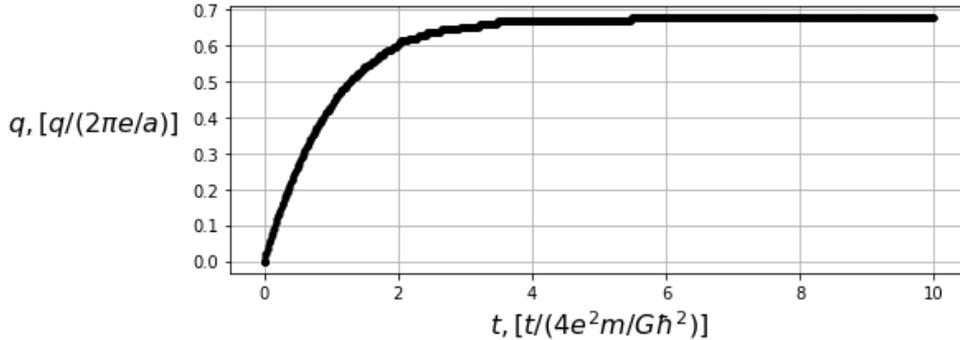
## 5.5 Solution to the quasicharge equation

With our newly calculated bandstructure, we can finally solve equation (49). In figure (9) we see the lowest bandstructure,  $E^{(0)}$ , which of course is essential to our solution. Please note, that in some of the plots, I plot as a function of  $k$ , and in some plots, I plot as a function of  $q$ . One could however easily go from  $k$  to  $q$ , and the other way around, by using the relation [7]  $q = 2ek$ .

We realise, by inspection of equation (49), that we are going to have two different solutions to the quasicharge. One where  $I \leq \max\left(G\frac{dE^{(0)}}{dq}\right)$  and one where  $I > \max\left(G\frac{dE^{(0)}}{dq}\right)$ . The quasicharge is solved numerically, in each of these cases, in figure (10) and figure (11). By comparison of the two figures, it is clear that when  $I$  is large, the quasicharge gets driven over the steepest parts of the bandstructure. When  $I$  is small however, the quasicharge goes asymptotically against the value of  $q$  that satisfies the equation  $I = G\frac{dE^{(0)}}{dq}$ .

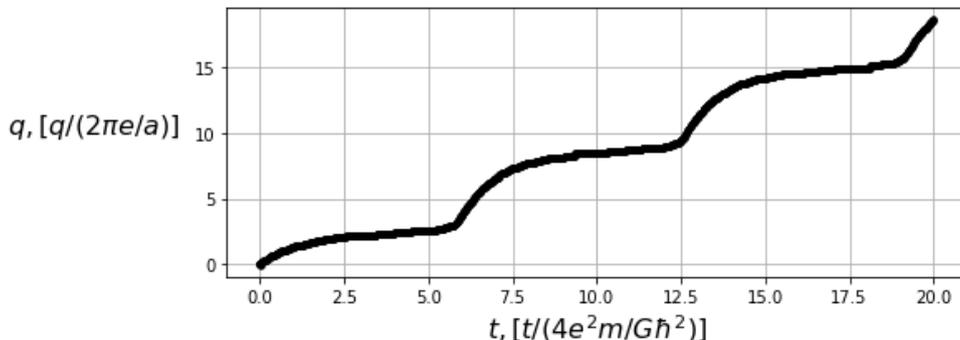


**Figure 9:** The lowest bandstructure.  $E_J = 3\frac{\hbar^2 k^2}{2m}$



**Figure 10:** Solution to the quasicharge for  $I = 1 \frac{\hbar^2 q}{4e^2 m}$ .

This means that  $I \leq \max \left( G \frac{dE^{(0)}}{dq} \right)$



**Figure 11:** Solution to the quasicharge for  $I = 2.1 \frac{\hbar^2 q}{4e^2 m}$ .

This means that  $I > \max \left( G \frac{dE^{(0)}}{dq} \right)$

## 5.6 Small, AC-driven Josephson junctions

So far, when solving equation (48), we have assumed the driving current to have no time-dependence. We have thus assumed a DC case, i.e.  $I(t) = I_0$ . One could however, easily drive the Junction with a mix of DC and AC:

$$I(t) = I_0 + I_A \cos(\omega t) \quad (58)$$

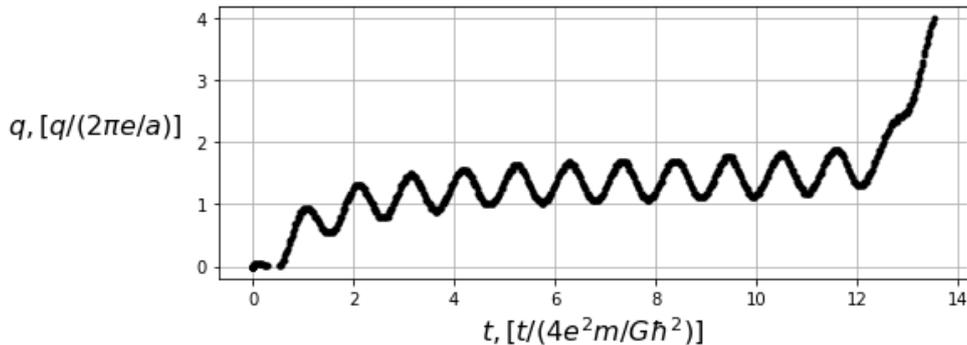
Here  $I_0$  is the DC part, and  $I_A$  is the AC amplitude.  $\omega$  is some frequency, in which the current alternates with. Examining equation (48) with the new time-dependent current, one quickly realises that we will have three new cases:

One where  $I(t)$  never grows to be larger than  $G$  times the largest slope of the bandstructure for all  $t$ , i.e.  $I(t) \leq \max(G \frac{dE^{(0)}}{dq})$ . This means the electron will be stuck in one part of the bandstructure, but still oscillate back and forth.

One where  $I(t)$  is larger than  $G$  times the largest slope of the bandstructure, for all  $t$ , i.e.  $I(t) \geq \max(G \frac{dE^{(0)}}{dq})$ . This corresponds to the direct current being solely able to make the electron travel along the bandstructure.

One where  $I(t)$  is not always larger than  $G$  times the largest slope of the bandstructure, i.e.  $I_0 + I_A > \max(G \frac{dE^{(0)}}{dq}) > I_0 - I_A$ . This corresponds to the electron only being

able to pass a top in the bandstructure, when the AC-part of the current aligns with the position of the electron, in such a way that  $I_A$  can push the electron "above the hill". One can imagine a situation where the electron has to oscillate for quite some time, before being able to pass to the next part of the bandstructure. This is shown in figure (12), with  $I_0 = 1.8 \frac{\hbar^2 q}{4e^2 m}$ , but with  $G \max(\frac{dE^{(0)}}{dq}) \approx 1.9 \frac{\hbar^2 q}{4e^2 m}$ , and  $I_A = 0.5 \frac{\hbar^2 q}{4e^2 m}$ . The quasicharge can only advance, when the AC-part is just right. This is shown in the oscillations in figure (12), before the big increment of quasicharge, at the end of the figure.



**Figure 12:** Quasicharge as a function of time in the small AC-driven Josephson junction.  $I_0 = 1.8 \frac{\hbar^2 q}{4e^2 m}$ ,  $I_A = 0.5 \frac{\hbar^2 q}{4e^2 m}$ ,  $\omega = 6 \frac{G\hbar^2}{4e^2 m}$ ,  $E_J = 3 \frac{\hbar^2 k^2}{2m}$

We now see, that even small changes in the current, can change the graph of the quasicharge, quite dramatically. This will turn out to have quite a big effect, when we calculate the I/V characteristics in the AC case.

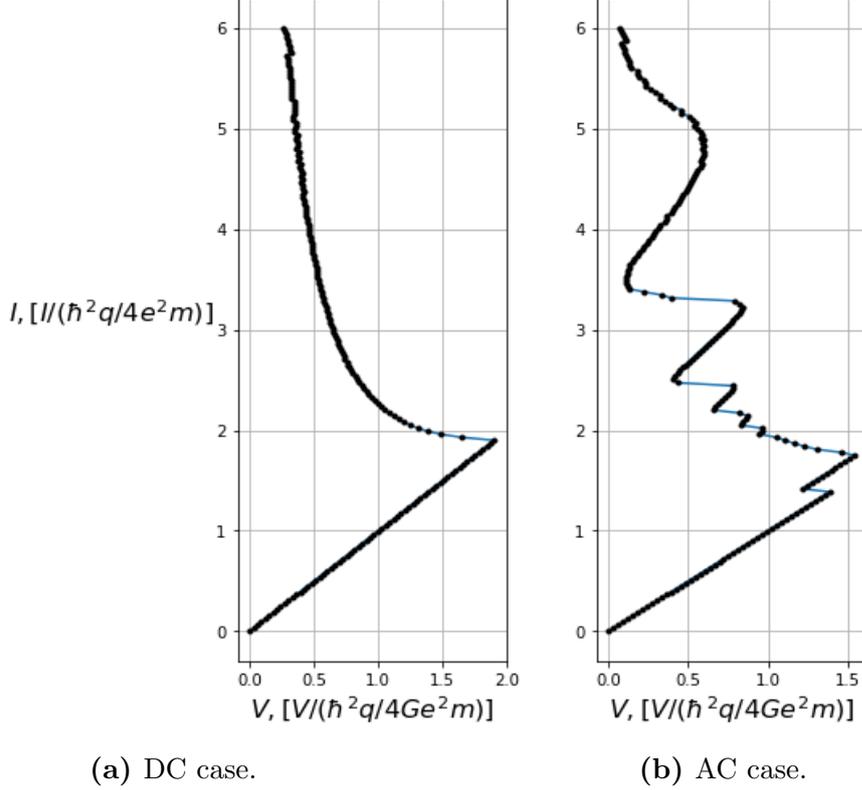
In the appendix, one will find a python script, which calculates the quasicharge, as a function of time. The script can take different values of  $I_0$ ,  $I_A$  and  $\omega$ , but is set to make a plot similar to figure (12).

## 5.7 I/V characteristics

Starting from equation (48), and using the relation [7]:  $V = dE^{(0)}/dq$ , we obtain an equation for the time-averaged voltage:

$$\bar{V} = \frac{1}{G}(\bar{I} - \bar{q}) \quad (59)$$

Where  $\bar{q}$  refers to the time-averaged change in quasicharge. Luckily, we have numerically calculated the quasicharge, for both the DC and AC cases, and are thereby able to calculate the voltage, as a function of current. The I/V characteristics can be seen in figure (13a) and figure (13b), for both the DC and AC cases respectively (the AC case refers to the case with an AC part included in the current, thus it is actually not purely AC driven, but rather a mix of DC and AC, see equation (58)).



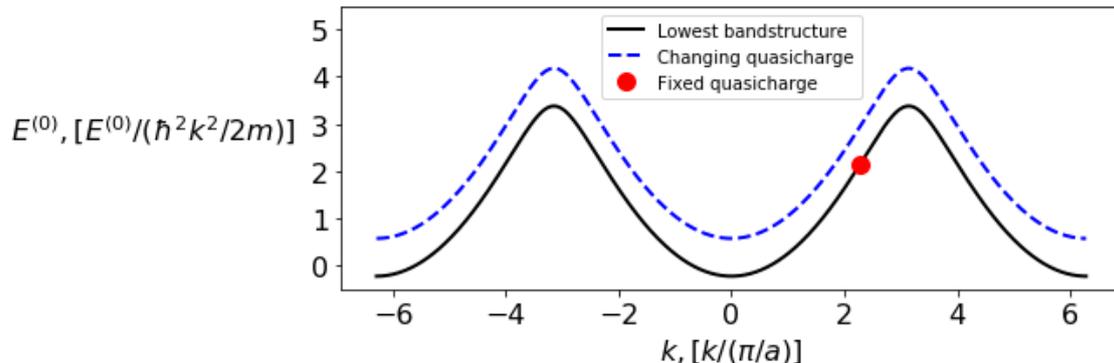
**Figure 13:** Numerically calculated I/V characteristics for small AC and DC driven Josephson junctions. Please note that it is both time-averaged current and voltage that is shown, and that the numerically calculated points are connected with a line. Both cases are with  $E_J = 3 \frac{\hbar^2 k^2}{2m}$ , and the AC case it with  $I_A = 0.5 \frac{\hbar^2 q}{4e^2 m}$ ,  $\omega = 6 \frac{G\hbar^2}{4e^2 m}$

As can be seen in figure (13a) and figure (13b), the I/V characteristics for both the DC and AC cases have some similar properties. For instance, the I/V characteristic is linear, until some point. While the I/V characteristic is linear, the electron must stay in a given part of the bandstructure, i.e.  $I \leq \max(GdE^{(0)}/dq)$ . When  $I$  is larger than  $G$  times the biggest slope of the lowest bandstructure, the electron is however no longer fixed in one place, and we see different behaviour on the I/V curves. These two different regimes are separated by the kink, on the I/V curves. The mathematical and physical interpretations are discussed below.

For the DC case,  $I \leq \max(GdE^{(0)}/dq)$  corresponds to figure (10), where it is clear, that the quasicharge moves asymptotically against some constant value. Therefore it is clear, that the time averaged change in quasicharge is zero, and thus we get a linear, ohmic relation:  $\bar{V} = (1/G)\bar{I}$ .

Physically, this can be understood by the non-zero commutator relation between the phase and the quasicharge,  $[\phi, q] = 2ei$ . When the quasicharge moves asymptotically against a fixed value, it becomes very well defined. This causes the phase, according to the commutator relation, to become completely undetermined. When the phase is undetermined, we have no supercurrent. This can be seen visually on the I/V curve, since we get a linear, ohmic current. When we have a well-determined quasicharge, we are in a Coulomb blocked state, and when we have well-determined phase, we are in a Bloch oscillating state [11]. The Coulomb blocked state corresponds to a state, in which the number of electrons in the junction is fixed, and thus the phase

undetermined. The Bloch oscillating state corresponds to a state where the number of electrons in the junction is completely undetermined, and the phase is thus determined. This is illustrated on the bandstructure, in figure (14)



**Figure 14:** Plot of the lowest bandstructure (dark line), with a given fixed quasicharge (red dot, corresponding to the Coulomb blockaded state). The dashed blue line symbolizes a changing quasicharge, corresponding to the Bloch oscillating state. Please note, that it should not be interpreted, as if the electron physically is on the dashed blue line, but rather that the dashed blue line symbolizes that the electron moves everywhere on the lowest bandstructure.

For the AC case,  $I \leq \max(GdE^{(0)}/dq)$  corresponds to the quasicharge oscillating back and forth in one part of the bandstructure, and thus the time-averaged change in quasicharge, will still be zero. Therefore we get the same ohmic relation, as in the DC case, as can be seen on the linear part of figure (13b). When we have  $I > \max(GdE^{(0)}/dq)$ , we also go from a Coulomb blockade to a Bloch oscillating state transition, as in the DC case. However, the transition will not be as sharp, due to the regime where the electron only occasionally is able to go above the top of each bandstructure, i.e.  $I_0 + I_A > \max(G \frac{dE^{(0)}}{dq}) > I_0 - I_A$ . Thus it makes excellent sense, that we see a more chaotic I/V curve, in the AC case, than in the DC case. We simply go back and forth between a Coulomb blockaded state and a Bloch oscillating state, because the electron will not always be able to pass the top of the band structure.

In both the DC and the AC case, we do however tend to see that an increase in current gives a drop in voltage. This makes physically excellent sense, because we get further and further into the Bloch oscillating regime. This means, that the more current applied to the circuit, the more of a Bloch oscillating state we have, and thus we get more super current. If we are to consider the RCSJ circuit in figure (2b), we can understand this behaviour better. At low currents, the Josephson junction is in a Coulomb blockaded state, and no supercurrent can run through the junction. Thus all the current, has to run through the resistance, and we get the usual ohmic behaviour. When the current is increased to the point where the Josephson junctions starts showing Bloch oscillating behaviour, some of the current will flow through the junction, as supercurrent, and thus less current has to run through the resistance. With less current through the resistance, we of course get a lower voltage on the circuit. This is why we see a drop in voltage, when we increase the current, in the I/V curves. The I/V curves thus simply show the transition between the Coulomb blockaded state to the Bloch oscillating state, of the Josephson junction.

## 6 Conclusion

In this bachelor thesis, I have investigated the physics of Josephson junctions. By considering Ginzburg-Landau theory in basic Josephson junctions, I have found an expression for the current over the junction, and free energy of the junction. With these expressions, I have derived many of the characteristics for circuits, involving Josephson junctions. The I/V characteristic for the overdamped RCSJ model can for instance be seen In figure (4). It turns out that the circuits described in this thesis, have very close mechanical analogs in the 'particle on a tilted washboard' and the 'mechanical pendulum' models. The similarities between the circuits and their mechanical analogs have been examined. With all these qualities derived, I started my examination of small Josephson junctions. With quantum mechanics taken into account, I found a differential equation for the quasicharge. With a numerical calculation of the bandstructure, I was able to make another numerical calculation of the time averaged voltage. Thus I reached the I/V characteristics, for both the purely DC-driven, small junction, and the mixed DC and AC-driven, small junction. I realised, that changing the current over the junction, one can make the junction change between a Coulomb blockaded state, and a Bloch oscillating state. The I/V characteristics are especially important for practical applications, because you have to understand the behaviour of electrical components in order to use them effectively.

## References

- [1] J R Waldram. *Superconductivity of metals and cuprates*. Institute of Physics Publishing, 1996.
- [2] Michael Tinkham. *Introduction to Superconductivity*. McGraw-Hill, Inc., second edition, 1996.
- [3] Thorvald Wadum Larsen. *Mesoscopic Superconductivity towards Protected Qubits*. PhD thesis, 2018.
- [4] Brian Møller Andersen. Condensed matter physics 2 (pdf), 2017.
- [5] Ginzburg-landau theory. [https://en.wikipedia.org/wiki/Ginzburg%E2%80%93Landau\\_theory](https://en.wikipedia.org/wiki/Ginzburg%E2%80%93Landau_theory). Accesed: 03-05-2019, at 11:15 am.
- [6] Antonio Barone and Gianfranco Paternò. *Physics and applications of the Josephson effect*. John Wiley Sons, Inc., 1982.
- [7] K. K. Likharev and A. B. Zorin. Theory of the bloch-wave oscillations in small josephson junctions. *Journal of Low Temperature Physics*, Vol. 59, 1985.
- [8] Fardin Kheirandish. Open quantum systems in heisenberg picture.
- [9] Henrik Bruus and Karsten Flensberg. *Many-Body Quantum Theory in Condensed Matter Physics*. Oxford university press, 2004.
- [10] Charles Kittel. *Introduction to Solid State Physics*. John Wiley Sons, Inc, eighth edition, 2005.

- [11] René Lindell, Laura Korhonen, Antti Puska, and Pertti Hakonen. Modeling and characterization of bloch oscillating junction transistors. 2009.

# Appendices

## A Python script calculating the bandstructure and quasicharge as a function of time

The python script below, calculates the bandstructure, for  $N = 11$  equations in the eigenvalue problem. It then takes the lowest bandstructure, and numerically calculates the quasicharge. In this script, I have put  $I_0 = 1.8$ ,  $I_A = 0.5$ , and  $\omega = 6$ . This can of course be changed, to the liking of the person running the script (in order to plot the DC-case, just put  $I_A = 0$ ).

```

1 import numpy as np
2 import matplotlib.pyplot as plt
3
4 m = 1; a = 1; hbar = 1; E_J = 3 #Defining my constants
5 N = 11 #N is the number of equations in my eigenvalue problem
6 n = 500 #n is number of elements in my bandstructure
7 Liste = np.zeros((n,N)) #Liste is an empty matrix, which i will put my
   bandstructure into
8 lambda_k = np.zeros(N) #lambda_k is another empty list, which I whill
   fill out
9 A = np.zeros((N,N)) #A is again an empty matrix, which I will fill out
10 for i in range(N-1): #Putting E_J/2 into A
11     A[i, i + 1] = E_J / 2
12     A[i + 1, i] = E_J / 2
13
14 k_ekstrem = 2 #k is the range of my k vektor.
15 k = np.linspace(-k_ekstrem*np.pi, k_ekstrem*np.pi, n)
16
17 G = ( 2*np.pi / a ) * np.linspace(-N/2 + 0.5, N/2 - 0.5, N) #Definition
   of G
18
19 for j in range(n): #Filling out lambda_k, and putting my solutions into
   Liste
20     for i in range(N):
21         lambda_k[i] = ( hbar**2 / (2*m) ) * (k[j] + G[i] )**2
22         A[i, i] = lambda_k[i]
23         Liste[j, :] = np.linalg.eig(A)[0][:]
24 Liste = Liste.T
25
26
27 plt.figure(figsize=(8,6)) #In this part of the code, I plot the
   bandstructure
28 plt.title('Bandstructure', fontsize = 16)
29 plt.xlabel('$k, [k / (\pi / a)]$', fontsize = 16)
30 plt.ylabel('$E, [E / (\hbar ^2 k^2 / 2m)]$', rotation = 0, fontsize = 16,
   labelpad = 65)
31 plt.xticks(fontsize=16)
32 plt.yticks(fontsize=16)
33 plt.grid()

```

```

34 for i in range(N):
35     plt.plot(k/np.pi, Liste[i], '.''k')
36
37 E = np.zeros((N*n,2)) #Now I define an empty matrix E, in which I put all
    my
38 for i in range(N): #bandstructures and their coresponding k-values in
39     E[i*n:i*n+n,0] = Liste[i]
40     E[i*n:i*n+n,1] = k
41
42 for i in range((N*n)-1,-1,-1): #Here I delete all bandstructures above a
    given value, because
43     if E[i,0] > 3.4: #Im only interested in the lowest bandstructure
44         E = np.delete(E, i, axis=0)
45
46 eps = np.zeros((int(E.size/2),2)) #Here I sort all k's in the
    bandstructure, so I get them
47 eps[:,1] = np.sort(E[:,1]) #in the right order
48 for i in range((int(E.size/2))):
49     for j in range((int(E.size/2))):
50         if E[j,1] == eps[i,1]:
51             eps[i,0] = E[j,0]
52 E = eps #I again save my lowest bandstructure in E
53
54 plt.figure(figsize=(8,6)) #Here I do a plot of the lowest bandstructure
55 plt.grid()
56 plt.xlabel('$k, [k / (1/a)]$', fontsize = 16)
57 plt.ylabel('$E, [E / (\hbar^2 k^2 / 2m)]$', rotation = 0, fontsize = 16,
    labelpad = 65)
58 plt.xticks(fontsize=16)
59 plt.yticks(fontsize=16)
60 plt.title('Lowest bandstructure', fontsize = 16)
61 plt.plot(E[:,1],E[:,0])
62
63 a = np.zeros(int((E.size/2) - 1)) #I find the slope between each point,
    and save these values in a
64 for i in range(a.size):
65     a[i] = (E[i+1,0] - E[i,0]) / (E[i+1,1] - E[i,1])
66
67 #Here I define my constants, for calculating the quasicharge
68 NN = 10; I_0 = 1.8; I_A = 0.5; omega = 6; V = np.zeros(NN); G = 1
69
70 #number is the amount of times i will test for a new value of q
71 number = int(E.size/2)*2
72
73 liste = np.zeros([2,number]) #I define some empty lists, which will be
    filled out later
74 summen = np.zeros(number)
75 t = np.linspace(0,20,number) #t is the time, which I will be integrating
    over
76
77 kk = 0 #Here i do my numerical integration!
78 for j in range(number):
79     for i in range(250,499,1):
80
81         if j == 0:
82             summen[j] = (I_A*np.cos(omega*t[1]) + I_0 - G*a[i])*t[1]
83
84         if j != 0:

```

```

85     summen[j] = I_A*(np.cos(omega*t[j]) - np.cos(omega*t[j-1]))
86     \
87     + (I_0 - G*a[i])*t[1] + summen[j - 1]
88     if round(E[i,1],1) == round(summen[j],1):
89         liste[:,kk] = [t[j],E[i,1]]
90         kk = kk+1
91         break
92
93 plt.figure() #Here I plot my quasicharge as a function of time
94 plt.figure(figsize=(8,3))
95 plt.xlabel('$t, [t/(4e^2 m / G \hbar ^2)]$', fontsize = 16)
96 plt.ylabel('$q, [q / (2 \pi e /a)]$', rotation = 0, fontsize = 16,
97         labelpad = 60)
97 plt.grid()
98 plt.plot(liste[0,:],2*liste[1,:]/(np.pi),'.',c='k')

```