Tuneable Long Range Interactions in an Array of coupled Cooper Pair Boxes

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Abstract

It was shown, that a Kitaev chain can be implemented in an array of superconducting islands with semiconducting nanowires. The system can be mapped on an Ising model. Adding capacitances between the superconducting islands introduces additional interactions in that Ising model. In this work we will search long range interactions in that system in order to be able to implement a long range Ising model in a macroscopic system. We will use different techniques for that. First we are going to look at phaseslips in the path integral formalism, using analytical and numerical ways to solve for the instanton solution. Those calculations will suggest a long range interaction in a certain parameter regime of the system. The range of that interaction will be limited by the quotient of two capacities. Since we cannot find all prefactors required in the dilute gas approximation, we try to reproduce the results by doing perturbation theory on an approximated groundstate. We find a potential formed similar to the potential predicted by the path integral calculations.

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Chapter 1

Introduction

In physics there are different types of long range interactions. From condensed matter the Coulomb interaction, and related to that dipole-dipole interactions, or the Van-der-Waals interaction are well known examples. In many systems those interactions will be changed by an effective screening, for example the Thomas-Fermi screening [1]. There has been effort to find a system, with a tunable long range interaction. One approach is to use cold bosonic quantum gases [2]. The idea is, that such a system can be used to simulate other systems with long range interactions, or in some cases is even expected to be helpful for quantum information processing [3–5]. In this work, we will look at a system made of small superconducting islands called Cooper-pair boxes [6]. The possibility to build qubits using Cooper-pair boxes [7] shows a good potential concerning control and coherent dynamics of a system made of them. The Cooper-pair boxes will be coupled capacitively, which will induce charge interactions between them. It has been shown that this system can be manipulated, so it can simulate an interacting Ising model [8]. Finding long range charge interactions in that system would imply that this system is sufficient to run a quantum simulation of a long range Ising model. Therefore in this work we are going to calculate corrections to the groundstate energy due to additional charges on the superconducting islands of such a system. Those corrections yield the effective charge interaction. In this chapter we start out with an introduction to the system in sec. 1.1. Before we start working with that system we will take a look at a similar, but purely electrostatic system in sec. 1.2, because it shows why we expect long range charge interactions in the original system. In sec. 1.3 we derive the Lagrangian and Hamiltonian of the system, to be able to describe them mathematically. In chapter 2 we use Mathieu functions to find the groundstate energy of the Cooper-pair box as a point of reference to check the results from other calculations. In chapter 3 we do a step by step calculation of the corrections to the groundstate energy of the coupled Cooper-pair boxes. We start out with the groundstate energy of one Cooper-pair box without correction terms for an external voltage in sec. 3.1. In sec. 3.2 we calculate those corrections by including so called instanton solutions, which are solutions to the classical equation of motion, going from one potential minimum to another. In sec. 3.3 we generalize this idea to the system

of coupled Cooper-pair boxes. For that we will especially have to find instanton solutions in that system, which will require an approximation of the potential. In sec. 3.4 we will compare that to numerical instanton solutions to the exact potential, after briefly discussing the idea of the numerics that calculated those instantons. In chapter 4 we will start out with the Cooper-pair box in sec. 4.1 again. We will construct an effective low energy Hamiltonian to find the groundstate and use perturbation theory for the corrections to the groundstate energy. That approach will yield a groundstate approximation, that we will generalize to the system of coupled Cooper-pair boxes in sec. 4.2. We will compare the scaling of the resulting interaction with that of chapter 3.

1.1 Model

In this section we are going to introduce the system we are going to work with. The basic building block is the Cooper-pair box, which is a superconducting island with a capacity and a Josephson junction. The superconducting island has two important quantities to describe its state. One is the charge number. Note that in a superconductor the electrons paired up to Cooper-pairs. Each of those consists of two electrons and therefore has the charge $2e$, where e is the electron charge. On a normal superconducting island we therefore have an even number of electrons. We speak of a fixed parity on a superconducting island. The other quantity is the superconducting phase. The superconductor has an order parameter, that is a complex number. The phase of that order parameter is the superconducting phase. It has a physical meaning, because it is canonically conjugated to the charge number and has an important role in the Josephson effect[1]. The Josephson effect yields an energy contribution from the Josephson junction. A Josephson junction consists of two superconductors separated by a small tunneling barrier, i.e, an insulator. The Josephson effect yields an energy contribution depending on the phase difference of the two superconductors. A more detailed introduction to superconductivity can be found in Ref. [9]. So let us take a look at the system we are going to work with in Fig. 1.1 and the system, that can be used to simulate an Ising model in Fig. 1.2. The nanowires on top of the superconducting islands will give rise to so called Majorana edge states/Majorana fermions. For the understanding of that work it is enough to know that they can break the parity of the superconducting island. This is what we simulate in our system with the external charges, that will induce offset charges as we will see in sec. 1.3. An introduction to Majorana fermions in solid state systems is given in Ref. [10]. In both systems the interaction between charges on different islands is achieved by the capacitors between the superconducting islands.

[1] Technically only phase differences between two superconductors have a physical meaning and the phase difference of two superconductors connected by a Josephson junction is canonically conjugated to the charge $\int I dt$, where I is the electric current through the Josephson junction. But since a Cooper-pair box has no other lead to the superconducting island every charge that enters the island has to go through the Josephson junction. Therefore the charge on that island only differs from the integral by a constant amount.

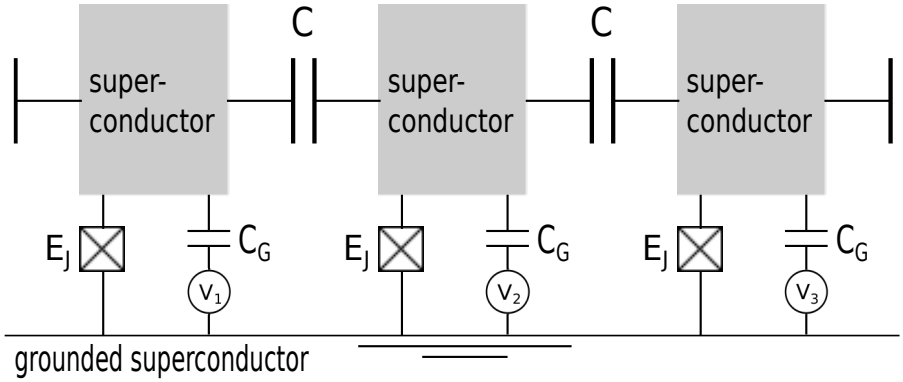

Figure 1.1: The system consists of a grid of superconducting islands. Each island is coupled to a grounded superconductor via a Josephson junction with Josephson energy E_J and to external voltages with a capacitor of capacitance C_G. Each island with its coupling to the grounded super conductor and the external voltage is a Cooper-pair box. Nearest neighbors in this array of Cooper-pair boxes are coupled by a capacitance C.

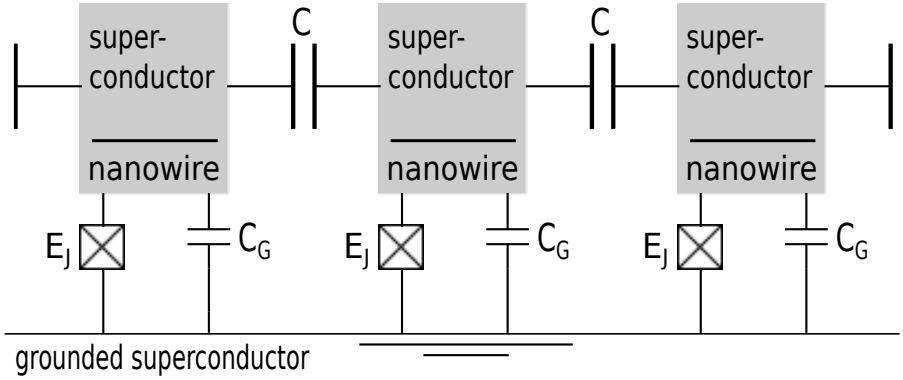

Figure 1.2: This is the system, that can be used to simulate an Ising model [8]. It is similar to 1.1, but has additional nanowires on top of the superconducting islands. We speak of topological Cooper-pair boxes here. The nanowires can break the islands parity, i.e, cause charge offsets, that interact with each other.

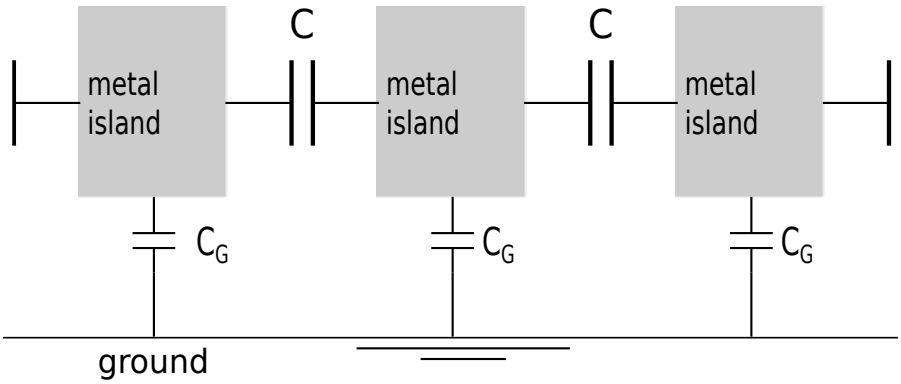

Figure 1.3: Here we have the same grid of capacitors as in Fig. 1.1, but no superconductors or Josephson junctions.

1.2 Yukawa Potential in a 1-d array of capacitors

Even though in our system in Fig. 1.1 all capacitors are between nearest neighbors, we want to look at the long range interactions. We will take a look at a similar purely electrostatic system to see that this is not a contradiction. Let us look at the system in Fig. 1.3.

The only quantities, that describe the state of this system are the charge numbers for each island. Without any nontrivial commutation relations we can describe the system with classical physics. We can then calculate the energy of the system by

$$E_{Cap} = \sum_{j=1}^{N} \frac{C_g}{2} U_j^2 + \frac{C}{4}(U_j - U_{j+1})^2 + \frac{C}{4}(U_j - U_{j-1})^2. \tag{1.1}$$

Here U_j is the voltage drop between Island j and the grounded superconductor. We simply summed up all energy contributions of all capacitors. In the classical system there are no other energy contributions. It is convenient to write this in terms of a capacitance matrix and charge/voltage vectors, where each entry of the vector is the charge/voltage on one island. Let us also introduce a dimensionless parameter $\eta = \frac{2C}{2C+C_G}$. Then we get

$$E_{Cap} = \frac{2C + C_G}{2} \boldsymbol{U}^\dagger C_M \boldsymbol{U} = \frac{2}{2C + C_G} \boldsymbol{Q}^\dagger C_M^{-1} \boldsymbol{Q} \tag{1.2}$$

with

$$C_M = \begin{pmatrix} 1 & -\frac{\eta}{2} & 0 & 0 & ... & -\frac{\eta}{2} \\ -\frac{\eta}{2} & 1 & -\frac{\eta}{2} & 0 & & \\ 0 & -\frac{\eta}{2} & 1 & -\frac{\eta}{2} & ... & \\ 0 & 0 & -\frac{\eta}{2} & 1 & ... & 0 \\ ... & & ... & ... & ... & -\frac{\eta}{2} \\ -\frac{\eta}{2} & & & 0 & -\frac{\eta}{2} & 1 \end{pmatrix}. \tag{1.3}$$

Since we are interested in charge interactions, we have to invert the capacitance matrix. To invert the matrix, let us first diagonalize it, because inverting

a diagonal matrix is simple. The eigenbasis can be guessed because of the translational-invariance of the system. We just have to do a Fourier series

$$\tilde{Q}_k = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{2\pi i \frac{k}{N} j} Q_j \tag{1.4}$$

$$\Rightarrow (\tilde{C}_M)_{k,k'} = \left(1 - \eta \cos\left(2\pi \frac{k}{N}\right)\right) \delta_{k,k'} \tag{1.5}$$

$$\Rightarrow (C_M^{-1})_{j,j'} = \frac{1}{N} \sum_{k=1}^{N} \frac{e^{2\pi i \frac{k}{N}(j'-j)}}{1 - \eta \cos\left(2\pi \frac{k}{N}\right)}. \tag{1.6}$$

For long range interactions long wave length dominate the behavior of the system. So in order to get the long range interaction, we can approximate the cosine term with a quadratic expansion, since only the short wavelength contributions are strongly underestimated. This approximation yields a one dimensional Yukawa potential

$$\Rightarrow (C_M^{-1})_{j,j'} \approx \frac{1}{N} \sum_{k=1}^{N} \frac{e^{2\pi i \frac{k}{N}(j'-j)}}{1 - \eta + \frac{2\eta\pi^2 k^2}{N^2}}. \tag{1.7}$$

For very large systems $N \to \infty$ this can be understood as a Riemann sum, so instead of a sum we can do an integral, that can be solved by a contour integration in the complex plane. We then get

$$(C_M^{-1})_{j,j'} \propto e^{-\sqrt{\frac{2}{\eta} - 2}|j-j'|}. \tag{1.8}$$

The step from a sum to an integral is a limit, that would make the system continuous. Therefore the prefactors would not be correct for the case of discrete islands, which is why we left them out. But the important insight from this is not the prefactor. It is the exponential decrease of charge interactions with distance and the fact that the decay length goes from zero to infinity as η goes from zero to one. That means we will always have an exponentially decreasing interaction, i.e, a screened interaction, since $\eta = 1$ should not be realizable in an actual experimental setup, because any stray capacitance would make $\eta < 1$. But that divergence of the decay length $\lambda = \sqrt{\frac{\eta}{2(1-\eta)}}$ shows that we can get an arbitrarily long decay length, if we get η close enough to one. In that sense we can talk about long range interactions. This System gives an example how the physics can be local in terms of voltages, but not in terms of charges. A qualitative explanation for those interactions is that each charged island induces charges on its neighbors, which induce charges on their neighbors so that the correlation between the charges on different islands is not only a nearest neighbor effect. In the $\eta \to 1$ limit we get a perfect correlation between neighbors, so that it does not decrease with distance. In the quantum system charge will not be a good quantum number though. That leaves the question whether there will still be a long range interaction.

1.3 Mathematical description of the Model

In the last section we have discussed a simpler system, that can be described by classical physics. In this section we will return to the coupled Cooper-pair boxes of Fig. 1.1. We will derive the Lagrangian and Hamiltonian of the system. The Hamiltonian will clarify the idea of charge offsets mentioned before. In the end there will be a brief discussion which parameter region of the system we are interested in. Let us start with the capacitive energy again. Remember that this time we have external voltages, that contribute to the energy

$$E_{Cap} = \sum_{j=1}^{N} \frac{C_g}{2}(U_j - V_j)^2 + \frac{C}{4}(U_j - U_{j+1})^2 + \frac{C}{4}(U_j - U_{j-1})^2. \tag{1.9}$$

The other energy contribution is due to the Josephson effect

$$V(\Phi_j) = E_J \sum_{j=1}^{N}(1 - \cos(\Phi_j)). \tag{1.10}$$

Here Φ_j is the difference of the superconducting phases of Island j and the grounded superconductor. Those two energy contributions can be used to construct the Lagrangian. To do that we need the first Josephson relation

$$U = \frac{\hbar}{2e}\dot{\Phi}. \tag{1.11}$$

That relation implies, that the capacitive energy can be understood as the kinetic energy of the dynamics of the superconducting phases

$$E_{cap} = \sum_{j=1}^{N} \frac{\hbar^2}{16E_C}(\dot{\Phi}_j^2 - \frac{\eta}{2}(\dot{\Phi}_j\dot{\Phi}_{j+1} + \dot{\Phi}_j\dot{\Phi}_{j-1})) - \frac{\hbar C_g V_j}{2e}\dot{\Phi}_j + \frac{C_g}{2}V_j^2, \tag{1.12}$$

where $E_C = \frac{2e^2}{C_G}$. Now we have a kinetic energy and Eq. (1.10) can be understood as the potential depending on our dynamic variables Φ_j. The construction of a Lagrangian is straight forward

$$L = \sum_{j=1}^{N} \frac{\hbar^2}{16E_C}\left(\dot{\Phi}_j^2 - \frac{\eta}{2}\left(\dot{\Phi}_j\dot{\Phi}_{j+1} + \dot{\Phi}_j\dot{\Phi}_{j-1}\right)\right) - \underbrace{\frac{\hbar C_g V_j}{2e}}_{\frac{q_j\hbar}{2e}}\dot{\Phi}_j + \frac{C_g}{2}V_j^2 - E_J(1-\cos(\Phi_j)) \tag{1.13}$$

$$\Rightarrow L = \sum_{j=1}^{N}\left(\sum_{j'=1}^{N}\frac{\hbar^2}{16E_C}\dot{\Phi}_j(C_M)_{j,j'}\dot{\Phi}'_j\right) - \frac{\hbar q_j}{2e}\dot{\Phi}_j + \frac{C_g}{2}V_j^2 - E_J(1-\cos(\Phi_j)). \tag{1.14}$$

This Lagrangian already describes the dynamics of the system. But it is still useful to derive the Hamiltonian. To do that we will have to find the momentum $Q_j = \frac{\partial L}{\partial \dot{\Phi}_j}$, which we can identify as the charge number on each island, because

as mentionend before, in superconductors charge is the quantity canonically conjugated to the superconducting phase, i.e, the momentum [9]. Note that the unit of that operator is convention dependend. In our case we could call it the Cooper-pair number operator, which gives dimensionless numbers. From classical physics we know

$$H = \left(\sum_{j=1}^{N} \frac{\partial L}{\partial \dot{\Phi}_j} \dot{\Phi}_j \right) - L \tag{1.15}$$

$$\Rightarrow H = \sum_{j=1}^{N} \left(\sum_{j'=1}^{N} 4E_C (C_M)^{-1}_{j,j'} (Q_j - q_j/2e)(Q_{j'} - q_{j'}/2e) \right) + E_J(1 - \cos(\Phi_j)). \tag{1.16}$$

Here we can see how the external voltages induce offset charges. Now that we have the framework to calculate the systems interactions, we need to discuss the parameter region we are interested in. We will look at systems with $\frac{E_J}{EC} \gg 1$, because we want the phase to be pinned to zero, which is important for the idea to implement an Ising model in the system. We are also going to choose η to be large i.e. close to one, because the system is well known for small η already [8]. Otherwise one also would not expect long range interactions. Not even in the classical system, as we have seen. The absolute magnitude of E_J and E_C is not important for the range and the form of the interaction in the system.

Chapter 2

Cooper Pair Box

In this section we will use Mathieu equations, to solve for the groundstate energy and following from that the charging energy of a single Cooper pair box. This will serve as a point of reference, to which we can compare results from other calculations. This will give an idea of how well and in which region of $\frac{E_J}{E_C}$ those calculations work. From Eq. (1.16) we can get the Hamiltonian for one Cooper-pair box

$$H = 4E_C(i\partial_\Phi - q/2e)(i\partial_\Phi - q/2e) + E_J(1 - \cos(\Phi)). \tag{2.1}$$

Note that the charge operator is expressed by a derivative with respect to Φ. We can now see that a gauge transformation cancels the charge offset $\Psi(\Phi) \rightarrow e^{-iq\Phi/2}\Psi(\Phi)$. It is important to note that such a gauge transformation changes the boundary conditions. It has a phase factor $e^{i\pi q/e}$, which is $2e$ periodic in q. Therefore we expect the eigenenergies to be $2e$ periodic in q as well. After the gauge transformation the eigenvalue problem results in a Mathieu equation. Those have been studied intensively and are implemented in most numeric/algebra programs. Therefore it is simple to get the groundstate energy E_0 and its dependence on q. In Fig. 2.1 and Fig. 2.2 we can see that the groundstate energy approaches a cosine like dependence on the offset charge q for large $\frac{E_J}{E_C}$. For small $\frac{E_J}{E_C}$ the groundstate energy approaches a parabola, as one would expect in a classical system. As expected in both cases the groundstate energy is $2e$ periodic, due to the periodicity of the boundary condition. The more physical explanation is, that in a superconductor the charge is quantized in units of $2e$. Therefore a charge offset of $2e$ can be compensated and does not change the groundstate energy. We will very much focus on the dependence of the Energy splitting/charging energy due to q i.e. $E_0(q = e) - E_0(q = 0)$ as a function of $\frac{E_J}{E_C}$, because in the following calculations the expected cosine like behavior of E_0 as a function of q is very generic and does not need to be tested again. In our calculations in the following chapters this cosine term will be a first order correction. As we can see this is enough for our regime of $E_j \gg E_C$. In the many island system in Fig. 1.1) we will need to find similar terms with an energy splitting as a function of the distance of two charges, since we are interested in their interaction. The correct results for a single Cooper pair box are in shown in Fig. 2.3.

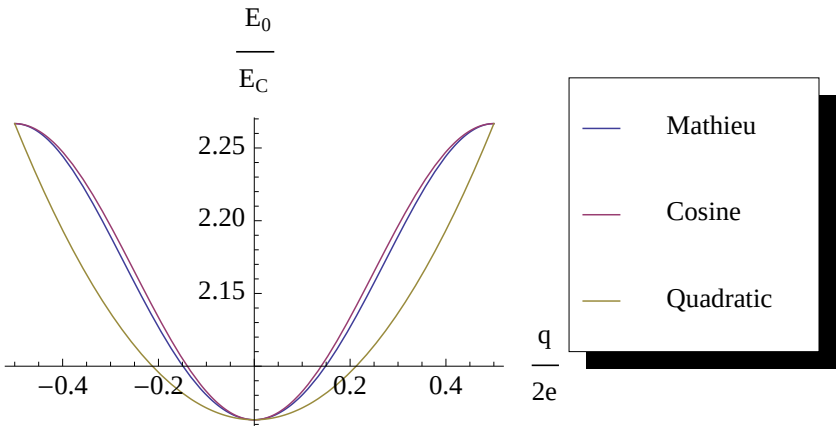

Figure 2.1: We have plotted the groundstate energy of a Cooper pair box with $\frac{E_J}{E_C} = 3$ depending on q, calculated from Mathieu equations. As as comparison we have also plotted a cosine like, and a parabolic graph, with the same energy splitting. In the $E_J \gg E_C$ regime, the groundstate energy has a cosine like dependence on the offset charge.

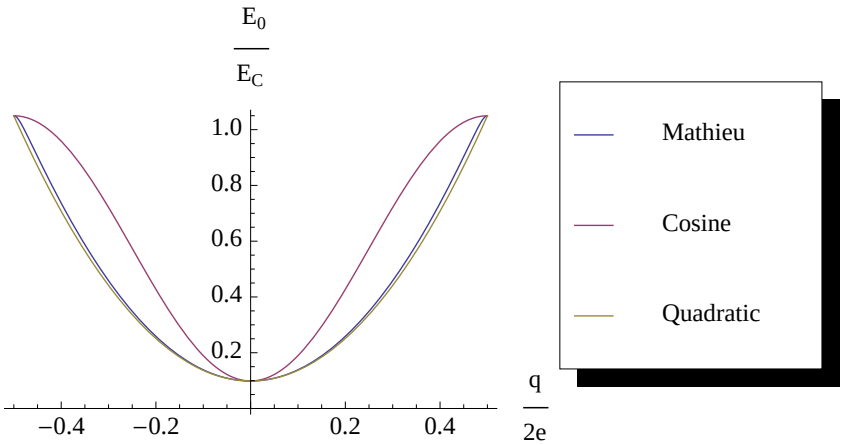

Figure 2.2: Like Fig. 2.1, but $\frac{E_J}{E_C} = 0.1$. The weak Josephson effect almost makes the system a simple capacitor, therefore the graph of the groundstate energy dependence on the offset charge is almost parabolic.

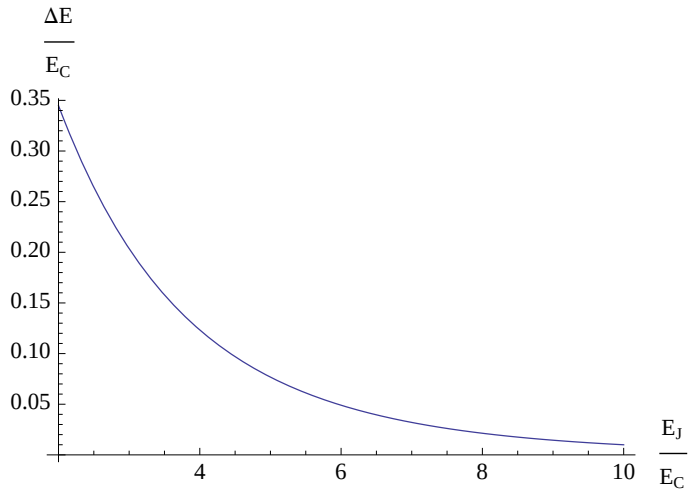

Figure 2.3: Here we plotted the energy splitting $\Delta E = E_0(q = e) - E_0(q = 0)$ of a single Cooper box as a function of $\frac{E_J}{E_C}$.

Chapter 3

Effective interaction via path integrals

The path integral formalism can be used to find the matrix elements of the time development operator between any two position eigenstates $|\Phi''\rangle$ and $|\Phi'\rangle$ with arbitrary time difference T. We are going to use imaginary times T to find the groundstate energies. To understand how we do that, let us look at such a matrix element and do a spectral decomposition of the time development operator with $|\Psi_n\rangle$ as the energy eigenstates with eigenvalue E_n

$$\langle\Phi''|e^{-HT/\hbar}|\Phi'\rangle = \sum_n \langle\Phi''|\Psi_n\rangle e^{-E_n T/\hbar}\langle\Psi_n|\Phi'\rangle. \tag{3.1}$$

The term, that decays the slowest in that sum, is the term with the lowest energy E_n. Therefore that term dominates the sum in the $T \to \infty$ limit, assuming $\langle\Phi''|\Psi_0\rangle\langle\Psi_0|\Phi'\rangle \neq 0$, where $|\Psi_0\rangle$ is the groundstate. Thus we obtain the groundstate energy via

$$E_0 = -\lim_{T\to\infty}\left[\log(\langle\Phi''|e^{-HT/\hbar}|\Phi'\rangle)\frac{\hbar}{T}\right]. \tag{3.2}$$

In this chapter we are going to do a step by step calculation of the dependence of the groundstate energy of the system in Fig. 1.1 on the offset charges. To do that we are going to start with the calculation of the groundstate energy of a harmonic oscillator, and then include correction terms to get the groundstate energy of the Cooper pair box. Those will depend on the offset charge. With that knowledge of the formalism and the approximations we made to get that correction term, we are going to move on to the interacting system and calculate correction terms depending on two charges, which yield the effective interaction between two charge offsets. In this calculation we will have to solve the classical equation of motion. We will do that analytically and numerically and compare the results. The path integral techniques applied in this section follow the discussion on path integrals in Ref. [11].

3.1 Groundstate energy of the Cooper pair box

In this section we are going to calculate the groundstate energy of the Cooper pair box using path integrals. For path integrals we need a Lagrangian, which was derived in the first chapter, to calculate the action $S[\Phi(t)]$ of a path $\Phi(t)$. Since we are using imaginary times we need to calculate the dimensionless Euclidean action $S[\Phi(t)] = \int_{-T/2}^{T/2} L_E[\Phi(t)]dt/\hbar$. For the calculation in imaginary time we use a changed Lagrangian L_E. To get that we have to change the sign of the Lagrangian and change $t \to -it$, hence

$$L_E = \frac{\hbar^2}{16E_C}\dot{\Phi}^2 + i\frac{q\hbar}{2e}\dot{\Phi} - \frac{C_g}{2}V^2 + E_J(1-\cos(\Phi)). \tag{3.3}$$

From now on we will drop out the term $-\frac{C_g}{2}V^2$, because it only shifts the energy by a constant amount. In the long run we are interested in the correction terms due to the charge offset, which is not affected by a constant energy shift. The term $i\frac{q\hbar}{2e}\dot{\Phi}$ is a geometric phase. Its contribution is completely imaginary and depends only on the start and end point of a path. The formula for a matrix element of the time development operator [1]

$$\langle\Phi''|e^{-HT/\hbar}|\Phi'\rangle = \int_{\substack{\Phi(-T/2)=\Phi' \\ \Phi(T/2)=\Phi''}} [D\Phi(t)]e^{-S[\Phi(t)]}, \tag{3.4}$$

shows that such an imaginary contribution does not make a path more or less likely. It can only cause interference effects. That is why geometric phases drop out of classical equations of motion. To find the groundstate energy we still have to choose an explicit matrix element, because so far Φ' and Φ'' are still variables. We will look at $\Phi' = \Phi'' = 0$, because the potential minimum is there so we can assume $\langle\Phi''|\Psi_0\rangle\langle\Psi_0|\Phi'\rangle \neq 0$ as required before and it should keep the calculation as simple as possible. Let us choose a dimensionless timescale $t' = E_J t/\hbar$ and $T' = E_J T/\hbar$. Then $S[\Phi(t')] = \int_{-T'/2}^{T'/2}\left[\frac{E_J}{16E_C}\dot{\Phi}^2(t') + 1 - \cos(\Phi(t'))\right]dt' + \frac{iq}{2e}(\Phi(T'/2) - \Phi(-T'/2))$. Note that for $\Phi' = \Phi'' = 0$ the geometric phase is zero. In order to evaluate this path integral, we are going to make a quasi classical expansion. That means we are going to solve the classical equation of motion

$$\frac{E_J}{8E_C}\ddot{\Phi}(t') = \sin(\Phi(t')) \tag{3.5}$$

and develop the action to second order around that solution. Note that the first order is zero in a solution of the classical equation of motion. We can see that $\Phi_0(t') = 0$ solves the equation of motion with the boundary conditions $\Phi(-T'/2) = \Phi(T'/2) = 0$ and has $S_0 = S[\Phi_0] = 0$. We are now going to split the paths $\Phi(t')$, that we integrate over in a sum of the classical solution

[1] In this equation we did not take the normalization factor into account, that is necessary to normalize this infinitely dimensional integral. So the equations concerning a matrix element calculated by the path integral formalism only express a proportionality. It is important though, that the proportionality factor is independent of t. Therefore we can only use the scaling of such a matrix element with t. Ref. [11] and [12] give more information on those normalizations.

plus a variation $\Phi(t') = \Phi_0(t') + \delta\Phi(t')$. Such a variation has the boundary condition $\delta\Phi(-T'/2) = \delta\Phi(T'/2) = 0$. This might seem pointless, because the classical solution here is $\Phi_0(t') = 0$, but in general the solution to the classical equation of motion can be different. Developing the action to second order in the variation yields

$$S \approx S_0 + \int_{-T'/2}^{T'/2} \delta\Phi(t') \left[-\frac{E_J}{16E_C}\partial_{t'}^2 + \frac{1}{2}\cos(\Phi_0(t')) \right] \delta\Phi(t')dt'. \tag{3.6}$$

That is the semi classical approximation. The operator acting on the variation of the path is the second variation of the action. In this case this approximation makes the problem a harmonic oscillator, because the development of the action included developing the potential to second order, i.e, a quadratic potential. This is why we also require $E_J \gg E_C$ for the path integral, because otherwise large variations, for which that approximation of the potential would be bad, would not pick up enough action, to be suppressed strong enough. Now that the action is quadratic in the variations, the path integral is a Gaussian integral. We know Gaussian integrals over D-dimensional vector spaces $\int \exp(-\pi \boldsymbol{v}^T O \boldsymbol{v}) d\boldsymbol{v} = \sqrt{\frac{1}{\det(O)}}$, where O is a $D \times D$ matrix. We are going to use this formula for the second variation of the action as well, even though it is an infinite dimensional operator. But in order to be able to use that formula, we have to define the measure of the path integral in analogy to the finite dimensional case, where we parameterize the integration space using an orthonormal basis. So if $\delta\Phi_n(t')$ is a complete orthonormal basis of all variations, which means $\int_{-T'/2}^{T'/2} \delta\Phi_n(t')\delta\Phi_{n'}(t')dt' = \delta_{n,n'}$, and $\Phi(t') = \Phi_0(t') + \sum_n \delta\Phi_n(t')c_n$, where c_n are parameters, then the measure looks like this

$$[D\Phi(t')] = \prod_n dc_n. \tag{3.7}$$

Then we can write the path integral in terms of a determinant

$$\langle 0|e^{-HT/\hbar}|0\rangle = \frac{e^{-S_0}}{\sqrt{\det(-\frac{E_J}{16\pi E_C}\partial_{t'}^2 + \frac{1}{2\pi}\cos(\Phi_0(t')))}}. \tag{3.8}$$

A determinant of such a differential operator can be evaluated by the Gelfand-Yaglom formula. For this formula we have to define a function $\Phi_{GY}(t')$, which is an eigenfunction to that operator with eigenvalue zero, but with the boundary condition $\Phi_{GY}(-T'/2) = 0$ and $\dot{\Phi}_{GY}(-T/2) = 1$. Then

$$\left[\det\left(-\frac{E_J}{16\pi E_C}\partial_{t'}^2 + \frac{1}{2}\cos(\Phi_0(t')) \right)^{-\frac{1}{2\pi}} \right] = \Phi_{GY}^{-\frac{1}{2}}(T'/2). \tag{3.9}$$

With $\cos(\Phi_0(t')) = 1$ we can solve that explicitly and get the result $\Phi_{GY}(t') = \sqrt{\frac{E_J}{8E_C}} \sinh\left(\sqrt{\frac{8E_C}{E_J}}(t' + T'/2) \right)$. Since we are interested in the groundstate energy, we need the scaling for large T', where the sine hyperbolic term is domi-

nated by one exponential

$$\begin{aligned}\langle 0|e^{-HT/\hbar}|0\rangle &\approx \left(\frac{E_J}{8E_C}\right)^{-\frac{1}{4}} \exp\left(-\sqrt{\frac{2E_C}{E_J}}T'\right) \\ &= \left(\frac{E_J}{8E_C}\right)^{-\frac{1}{4}} \exp\left(-\sqrt{2E_JE_C}\frac{T}{\hbar}\right).\end{aligned} \tag{3.10}$$

Therefore we can use Eq. (3.2) and get the groundstate energy of the system $E_0 = \sqrt{2E_JE_C}$. This is the result for a harmonic oscillator known from wave mechanics, just as we expected earlier. We calculated this in the path integral formalism, because now it is easier to calculate correction terms due to the periodic potential, that is not really quadratic.

3.2 Corrections to the groundstate energy

In the last section we have solved the classical equation of motion with the boundary condition $\Phi_0(-T'/2) = \Phi_0(T'/2) = 0$. Since Φ is the phase of the superconducting order parameter, it is 2π-periodic. We did not take that into account in the last section. So we should also have solved the classical equation of motion for boundary conditions $\Phi_0(-T'/2) = 0$ and $\Phi_0(T'/2) = 2\pi n$ with $n \in \mathbb{Z}$, made the quasi classical approximation around them, and then added up all those contributions. Note that n is a winding number [13]. In this case it counts how many times the path of the superconducting order parameter wound around zero in the complex plain. Let us now look at the solution to the classical equation of motion for $n = 1$ and calculate the corresponding contributions to the path integral. We can see that

$$\Phi_{1+}(t') = 4\arctan\left[\exp\left(\sqrt{\frac{E_J}{8E_C}}(t' - t'_0)\right)\right] \tag{3.11}$$

also solves the equation of motion[2] and has the desired boundary conditions for $T' \to \infty$. Here t'_0 is a free parameter due to time-translational invariance. In Fig. 3.1 we compare $\Phi_{1+}(t')$ to a numerical solution for finite T'. We can see that $\Phi_{1+}(t')$ is also a good approximation for instantons with finite $T' \gg \sqrt{\frac{8E_C}{E_J}}$. Now we proceed in analogy to the last section, that means we need the action of the classical path itself and we are interested in the integral over all variations, with the action developed to second order around that classical path again. Let us start with the action of the path itself. Here we can just plug the instanton solution $\Phi_{1+}(t')$ into the expression for the action and calculate the integral. If we do that we get

$$S[\Phi_{1+}(t')] = \sqrt{\frac{8E_J}{E_C}} + i\pi\frac{q}{e}. \tag{3.12}$$

[2]The fact that we get a solution to the classical equation of motion, that goes through the potential barrier might be confusing. It is important to remember that we are working with imaginary time and therefore with the Euclidean action, which caused the sign of the potential to change. Therefore the potential barrier is turned into well.

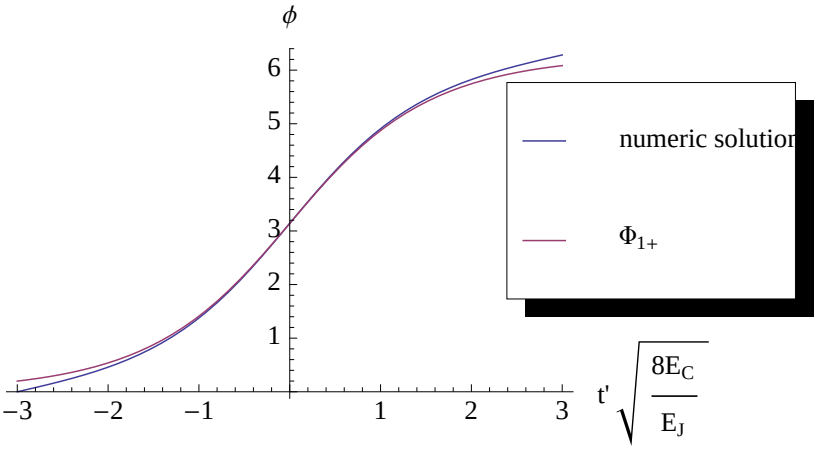

Figure 3.1: Here we plotted the instanton solution $\Phi_{1+}(t')$ and a similar numerical instanton solution for $T' = 6$.

After finding the action of that instanton solution, we need to find the second variation of the action around that solution and do the integral over all variations again. In analogy to the last section the second variation of the action around the instanton $\Phi_{1+}(t')$ is $-\sqrt{\frac{E_J}{16E_C}}\partial_{t'}^2 + \frac{1}{2}\cos(\Phi_{1+})$. Now we can express the path integral as a determinant again. This time we have to exclude one degree of freedom from the path integral and therefore from the determinant though. If we included all variations, we would also include the variation, that just slightly moves the tunneling event in time i.e. changes t_0'. That does not change the action, therefore this variation has the eigenvalue zero. With eigenvalue zero we cannot treat this variation as a Gaussian integral. Instead we will separately integrate over the parameter t_0' and define a determinant $\det'\left(-\frac{E_J}{16\pi E_C}\partial_{t'}^2 + \frac{1}{2\pi}\cos(\Phi_{1+})\right)$ as a determinant of the second variation of the action acting on the variations orthorgonal to the variation with eigenvalue zero. We will call that a reduced determinant from now on. To evaluate such a reduced determinant, we will evaluate it as if it was not reduced and then divide by the lowest eigenvalue[3]. In order to be able to solve the Gelfand-Yaglom equation we will approximate $\cos(\Phi_{1+})) \approx 1 - \sqrt{\frac{E_J}{2E_C}}\delta(t - t_0')$, which is an idea from normal scattering theory in wave mechanics, where scatterers are approximated as points, but the area under the potential is kept constant. Now we can solve the Gelfand-Yalgom equation. We already know the solution for $t' < t_0'$ from the discussion of the harmonic oscillator. At $t' = t_0'$ we get a jump condition for the slope of Φ_{GY} from the delta potential $\Phi_{GY}(t_0'^-) - \Phi_{GY}(t_0'^+) = \sqrt{\frac{E_J}{2E_C}}\Phi_{GY}(0)$. At $t' > t_0'$ the second variation of the action is exactly the same as in the last section again, so we can solve the differential equation there as well. We only have different boundary conditions there due to that jump in $t' = t_0'$. So for

[3]This eigenvalue will be zero in the $T' \to \infty$ limit, therefore we calculate the reduced determinant as a function of T' and then take that limit.

this instanton we get the solution to the Gelfand-Yaglom equation

$$\Phi_{GY}(t') = \begin{cases} \sqrt{\frac{E_J}{8E_C}} \sinh\left(\sqrt{\frac{8E_C}{E_J}}(t'+T'/2)\right) & t' < t'_0 \\ \sqrt{\frac{E_J}{32E_C}} \left(e^{\sqrt{\frac{8E_C}{E_J}}(t'+2t'_0-T'/2)} + e^{\sqrt{\frac{8E_C}{E_J}}(-t'-2t'_0+T'/2)}\right) & t' > t'_0 \end{cases}. \tag{3.13}$$

We can see that for this instanton we get $\Phi_{GY}(T'/2) = \sqrt{\frac{E_J}{8E_C}} \cosh \sqrt{\frac{32E_C}{E_J}} t'_0$. Since we have to evaluate a reduced determinant, we have to find the lowest eigenvalue of the second variaton of the action acting on all variations. For that eigenstate $\delta\Phi_0$, we use the ansatz[4]

$$\delta\Phi_0(t') = \begin{cases} \sqrt{\frac{E_J}{8E_C(1-\Delta)}} \sinh\left(\sqrt{\frac{8E_C}{E_J}(1-\Delta)}(t'+T'/2)\right) & t' < 0 \\ A\sqrt{\frac{E_J}{8E_C(1-\Delta)}} \sinh\left(\sqrt{\frac{8E_C}{E_J}(1-\Delta)}(-t'+T'/2)\right) & t' > 0 \end{cases} \tag{3.14}$$

with

$$A = \frac{\sinh\left(\sqrt{\frac{8E_C}{E_J}(1-\Delta)}(T'/2+t'_0)\right)}{\sinh\left(\sqrt{\frac{8E_C}{E_J}(1-\Delta)}(T'/2-t'_0)\right)} \tag{3.15}$$

where Δ is a parameter we have to choose, so that the jump condition is fulfilled. That leads to the equation

$$\begin{aligned} &\cosh\left(\sqrt{\frac{8E_C}{E_J}(1-\Delta)}(T'\right) \\ &= \sqrt{\frac{1}{1-\Delta}} \sinh\left(\sqrt{\frac{8E_C}{E_J}(1-\Delta)}(T'/2-t'_0)\right) \sinh\left(\sqrt{\frac{8E_C}{E_J}(1-\Delta)}(T'/2+t'_0)\right). \end{aligned} \tag{3.16}$$

This can be solved self consistently by approximating $\Delta T' \ll 1$. Then Δ can be calculated to be exponentially small in T'

$$\Delta \approx 4 \exp\left(-\sqrt{\frac{8E_C}{E_J}} T'\right) \cosh\left(\sqrt{\frac{32E_C}{E_J}} t'_0\right). \tag{3.17}$$

Therefore the approximation made here gets arbitrarily exact in the $T \to \infty$ limit. Note that the lowest eigenvalue of the second variation of the action is $\Delta/2\pi$. So now we have calculated everything we need, to evaluate that reduced determinant. We get

$$\det{}'\left(-\frac{E_J}{16\pi E_C}\partial_{t'}^2 + \frac{1}{2\pi}\cos(\Phi_{1+})\right) = \sqrt{\frac{E_J}{2\pi^2 E_C}} \exp\left(\sqrt{\frac{8E_C}{E_J}} T'\right). \tag{3.18}$$

So now we have found the reduced determinant, we have to do the integral over all tunneling times t_0. We already argued, that we are doing a change

[4] We ignore the normalization of the variation $\delta\Phi_0$ for now, because at this point we are only interested in the eigenvalue.

of integration variables from the amplitude of one variation to that tunneling time. Such a change of variables yields a Jacobi determinant. So in order to calculate that Jacobi determinant let us take a look at the variation $\delta\Phi_0(t')$, that moves an instanton in time. Since $\Phi_{1+}(t') + \partial_{t'_0}\Phi_{1+}(t')dt_0 = \Phi_{1+}(t' + dt'_0)$ for infinitisemal dt'_0, we know that $\partial_{t'_0}\Phi_{1+}(t')$ is a variation that moves $\Phi_{1+}(t')$ in time. Therefore $\delta\Phi_0$ has to be proportional to $\partial_{t'_0}\Phi_{1+}(t') = \partial_{t'}\Phi_{1+}(t')$, but still has to be normalized. Then we can get the Jacobi determinant from

$$\delta\Phi_0(t')dc_0 = \partial_{t'}\Phi_{1+}(t')dt'_0, \tag{3.19}$$

i.e, by finding the normalization factor for $\partial_{t'}\Phi_{1+}(t')$. That calculation yields $\frac{dc_0}{dt'_0} = \sqrt{\frac{8E_C\mathrm{Re}(S[\Phi_{1+}(t')])}{E_J}}$. Putting that factor and the reduced determinant together, the contribution of the instanton solution $\Phi_{1+}(t')$ to the matrix element $\langle 0|e^{-HT'/\hbar}|0\rangle$ is $\sqrt{\frac{E_J}{2\pi^2 E_C}}\exp\left(\sqrt{\frac{8E_C}{E_J}}T' + i\frac{\pi q}{e}\right)\int_{-T'/2}^{T'/2}\sqrt{\frac{8E_C\mathrm{Re}(S[\Phi_{1+}(t')])}{E_J\pi}}dt'_0$. So now we have evaluated the contribution to the path integral of the instanton with one tunneling event from 0 to 2π. The idea is to generalize this expression to the contributions for all instantons. Therefore we have to know what other instantons there are. Of course there also is an instanton tunneling down by 2π. Due to symmetry we can see, that the contribution of that instanton would be exactly the same, except for a different sign of the geometric phase, i.e, the imaginary part of the action. The problem is that there should also be instantons, that tunnel more than once. The difficulty here is that the instanton we were able to find analytically only approaches the potential minima in infinite time. Finding an instanton, that tunnels more than once analytically would be much more complicated. In order to find those we use the dilute gas approximation. There we simply add up solutions with single tunneling events, that are well separated in time. We will call the time when the m-th tunneling happens t'_m. The idea of that approximation is, that the equation of motion is local in time. At each tunneling event the dynamics are highly dominated by one single tunneling solution. So the equation of motion is fulfilled except for errors, that are exponentially small in the time difference between the two tunneling events.

In Fig. 3.2 we compare an approximated instanton and a numerically exact one. In Fig. 3.3 we have plotted an approximated instanton that is so complex that we can not easily find the boundary conditions to get a numerical exact analogue.

If we want to include all instantons, that we can construct like this, into our calculation, we have to calculate their actions and the path integral around each of them. We do not need to do this explicitly, but can generalize the results from the single tunneling instantons. Let us start with the action. We know the (real) action for one tunneling event $\mathrm{Re}(S[\Phi_{1+}(t')]) = \sqrt{\frac{8E_J}{E_C}}$. The (real) action of a tunneling instanton $\Phi_m(t')$ with m tunneling events then is $m\sqrt{\frac{8E_J}{E_C}}$, since the single tunneling events are well separated. We will call that S_m from now on. When we do the path integral for an instanton with m tunneling events, we now have to decrease the number of degrees of freedom by m, because we can not include the variations, that move any of the m tunneling events in time. We

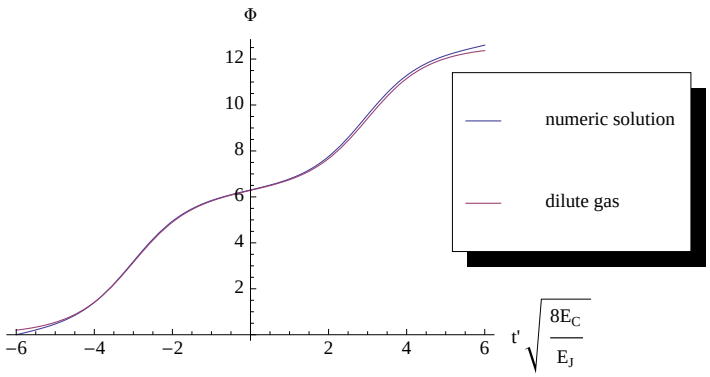

Figure 3.2: Here we plotted an analytically approximated instanton from the dilute gas approximation and a numerically exact instanton. The tunneling events are well separated on the scale dimensionless timescale $\sqrt{\frac{8E_C}{E_J}}$.

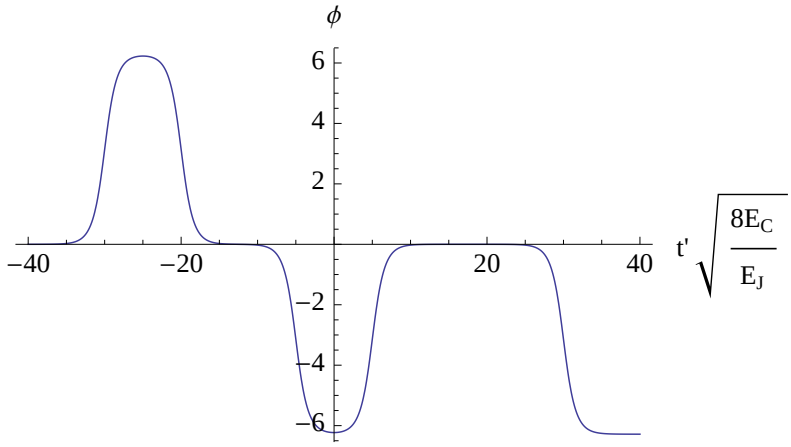

Figure 3.3: Here we plotted an approximated instanton with multiple tunneling events in both directions. Due to the separation of the single tunneling events the movement through the potential is the same as in the single tunneling event except for exponentially small corrections.

have already seen that one tunneling event only changes over all variations by a fixed factor in the $T' \to \infty$ limit. For many well separated tunneling events we can treat those as single tunneling events and get such a factor from each tunneling event, thus

$$\left(\frac{\det(-\frac{E_J}{16\pi E_C}\partial_t^2+\frac{1}{2\pi})}{\det'(-\frac{E_J}{16\pi E_C}\partial_t^2+\frac{1}{2\pi}\cos(\Phi_{1+}))}\right)^m = \frac{\det(-\frac{E_J}{16\pi E_C}\partial_t^2+\frac{1}{2\pi})}{\det'(-\frac{E_J}{16\pi E_C}\partial_t^2+\frac{1}{2\pi}\cos(\Phi_m))}. \quad (3.20)$$

That leaves only the factor due to the change of integration varibales. Since we have to change m integration variables now, we get that factor to the m. So now we can write down the sum over all instantons. To do that we sum over all numbers of tunneling events m and at each individual tunneling event over the possibilities of tunneling up or down

$$\langle 0|e^{-HT'/E_J}|0\rangle = \det\left(-\frac{E_J}{16E_C}\partial_t^2+\frac{1}{2}\right)^{-\frac{1}{2}} \sum_m \int \left(2F\cos\left(\frac{q\pi}{e}\right)\right)^m e^{-S_m} dt'_1 ... dt'_m \quad (3.21)$$

$$F = \left(\frac{8E_C S_1}{E_J} \underbrace{\left(\frac{\det(-\frac{E_J}{16E_C}\partial_t^2+\frac{1}{2})}{\det'(-\frac{E_J}{16E_C}\partial_t^2+\frac{1}{2}\cos(\Phi_{1+}))}\right)}_{2/\pi}\right)^{\frac{1}{2}}. \quad (3.22)$$

The cosine term in Eq. (3.21) is due to the interference of the instantons tunneling up or down. We did not explicitly write down the integration domains of the time integrals yet. In order to avoid double counting of instantons, we have to integrate $\int_{-T'/2}^{T'/2}\int_{t'_1}^{T'/2}...\int_{t'_{m-1}}^{T'/2} dt'_1 dt'_2 ... dt'_m = \frac{T'^m}{m!}$. Then we can do the sum over all m and get an exponential function

$$\langle 0|e^{-HT'/E_J}|0\rangle = \det\left(-\frac{E_J}{16E_C}\partial_t^2+\frac{1}{2}\right)^{-\frac{1}{2}} \exp\left(2F\cos(\frac{\pi q}{e})e^{-S_1}T'\right). \quad (3.23)$$

By using Eq. (3.2) we get the groundstate energy of a harmonic oscillator plus a correction term

$$E_0 = \sqrt{2E_J E_C} + \frac{2^{\frac{15}{4}}}{\pi^{\frac{1}{2}}} E_J^{\frac{3}{4}} E_C^{\frac{1}{4}} \cos\left(\frac{\pi q}{e}\right) e^{-S_1}. \quad (3.24)$$

Those energy corrections are already known from WKB calculations [14]. In Fig. 3.4 we compared these results to the known results from Mathieu equations.

3.3 Charge interactions

In the last section, we have seen how to calculate the groundstate energy of a Cooper pair box in the path integral formalism. Now we want to do that for large systems like in Fig. 1.1 and focus on groundstate energy corrections, that depend on two charges, i.e, induce an interaction. Just like in a single

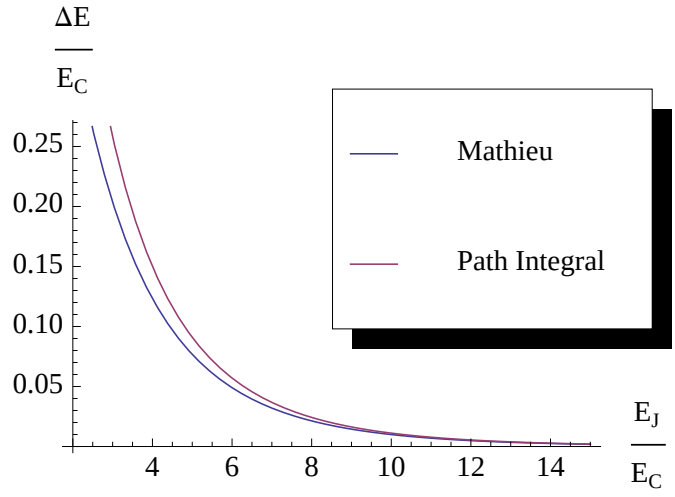

Figure 3.4: Here we plotted the groundstate energy splitting ΔE of the Cooper pair box due to the charge offset calculated bay path integrals. We compare that to the energy splitting known from Mathieu equations. In the regime where $E_J \gg E_C$, the path integrals results to coincide with those from the Mathieu equation. We would have expected that, because only in that limit it is possible to make the quasi classical approximation.

Cooper pair box, there are phase slips possible in that system. Since there are many Cooper pair boxes now, there is the possibility that phases tunnel simultaneously. The capacitive coupling makes that more likely than all those tunnelings happening by itself, as we will see later. What we are going to look at are instantons, where M neighbouring islands simultaneously tunnel in the same direction, because those events will induce the charge interactions. We will call that a tunneling cluster. Let us start with finding the instantons, and most important their actions. The Lagrangian was derived in sec. 1.3. We change it to the Euclidean Lagrangian in imaginary time again

$$L_E = \sum_{j=1}^{N} \left(\sum_{j'=1}^{N} \frac{\hbar^2}{16 E_C} \dot{\Phi}_j (C_M)_{j,j'} \dot{\Phi}'_j \right) + i \frac{\hbar q_j}{2e} \dot{\Phi}_j + E_J(1 - \cos(\Phi_j)). \qquad (3.25)$$

The problem is that there are interactions in this system. Therefore it is much more difficult to solve the equation of motion. For one Cooper pair box this was rather easy, because with energy conservation on classical paths we could break the problem down to one integral. In many dimensions we have more variables but not more known conserved quantities. We will find a way to approximate this problem through single particle physics, i.e, a non interacting problem though. In the classical system discussed earlier, we were able to use a Fourier series to diagonalize the capacitance matrix. In the quantum system we can still do that. The problem is, that this variable transformation leads to

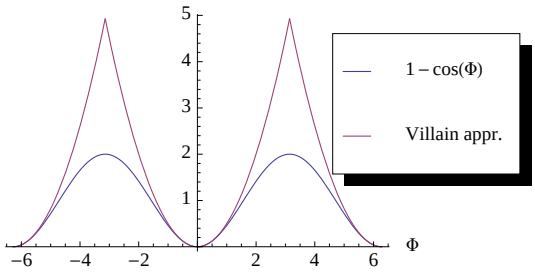

Figure 3.5: Here we plotted the dependence of the potential on the phase Φ and the Villain approximation of that term. In order to see the mistakes we made because of that approximation, we will do numerics in sec. 3.4.

an interacting potential

$$\tilde{\Phi}_k = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{2\pi i \frac{k}{N} j} \Phi_j \tag{3.26}$$

$$\Rightarrow V = \sum_{j=1}^{N} E_J (1 - \cos(\frac{1}{\sqrt{N}} \sum_{k=1}^{N} e^{-2\pi i \frac{k}{N} j} \tilde{\Phi}_k)). \tag{3.27}$$

In the Taylor series we can explicitly see those interactions, because we can do the sum over all j

$$\Rightarrow V = E_J \sum_{n=1}^{\infty} \sum_{k,k',\ldots k^{n\prime}} \frac{\tilde{\Phi}_k \tilde{\Phi}_{k'} \ldots \tilde{\Phi}_{k^{(n-1)\prime}} \tilde{\Phi}_{-k-k'-\ldots-k^{(n-1)\prime}}}{n! N^{n-1}}. \tag{3.28}$$

Note that the higher orders yield more than just two body interactions, which seems to make the problem very complicated. On the other hand the quadratic order does not yield an interaction at all, since $\tilde{\Phi}_k = \tilde{\Phi}^*_{-k}$. That makes the quadratic term depend only on one degree of freedom. The problem with approximating the cosine potential as a simple parabola became apparent in sec. 3.1 and 3.2. With only one minimum in the potential there are no phase slips and without phase slips there is no dependence of the groundstate energy on the charge offset. Therefore we will do a Villain approximation, where one approximates a negative cosine as a parabola around each minimum as can be seen in Fig. 3.5. In each locally parabolic potential there are no interactions, even in the new variables. But we get the problem of non trivial case distinctions in the new variables $\tilde{\Phi}_k$, which are the transformed variables introduced in Eq. (3.26). But let us first take a look at an analytic formulation of the Villain approximation in the old variables

$$V(\Phi_j) \approx \frac{E_J}{2} (\Phi_j - 2n_j\pi)^2, \qquad n_j \in \mathbb{N}, \quad -\pi < \Phi_j - 2n_j\pi \leq \pi. \tag{3.29}$$

We always have to choose n_j so that the requirements are fulfilled. These case distinctions will not be equations of single variables once we transform into

the new variables. In order to still be able to make that case distinction when solving for the instanton solution, i.e, make that case distinction before we have an explicit expression for the path, we will use symmetries. The system is time reversal, time translational, discretely translational invariant in $\mathbf{\Phi}$ and invariant under sign changes in $\mathbf{\Phi}$. So for an instanton solution with M islands tunneling simultaneously, i.e, $\mathbf{\Phi}_M(-T/2) = \mathbf{0}$ and $\mathbf{\Phi}_M(T/2) = 2\pi \sum_{j=r+1}^{M+r} \boldsymbol{e}_j$ where $\boldsymbol{e}_j$ are the unit vectors in dimension j and r is a parameter that changes which islands are tunneling, we can assume

$$\mathbf{\Phi}_M(-T/2+t) = -\mathbf{\Phi}_M(T/2-t) + 2\pi \sum_{j=r+1}^{M+r} \boldsymbol{e}_j. \tag{3.30}$$

The idea is that the identical potential minima are left/approached from different sides at different times, but the dynamics are the same except for the direction and point of time. This equation especially yields

$$\mathbf{\Phi}_M(0) = \pi \sum_{j=1}^{M} \boldsymbol{e}_j. \tag{3.31}$$

So at that point the instanton solution goes from one parabolic potential to the other. Now one might argue, that we do not know for sure, that there are not any other points of time, where at least one island jumps back and forth between the two sections. But since the border between two such sections is also a local potential maximum in at least one island, it is very unlikely, that the instanton solution will go through that border more than once. If one does not want to make that assumption, it is possible to take it as an upper bound approximation, since a missed case distinction would always result in an overestimated potential and therefore in a higher action. Eq. (3.30) also shows that it is enough to find the first half of the instanton solution i.e. in the time $T/2 < t < 0$, because the other half follows directly. Therefore we can just use one quadratic potential and find the solution of the equation of motion going from $\mathbf{\Phi}_M(-T/2) = \mathbf{0}$ to $\mathbf{\Phi}_M(0) = \pi \sum_{j=1}^{M} \boldsymbol{e}_j$. Since the quadratic potential does not yield any interactions after the variable transformation, we can now solve the problem as single particle physics in the new variables. Note that $\tilde{\Phi}_k$ is a complex number, which we can be split into $|\tilde{\Phi}_k|$ and its complex phase ϕ_k. So the dynamics of the complex phase could be important. Let us show, that in this case we can neglect them though. To do that, we write the Langrangian in the new variables with the approximated potential

$$L_E = \sum_{k=1}^{N} \frac{\hbar^2}{16 E_C} \left(1 - \eta \cos\left(2\pi \frac{k}{N}\right)\right) (|\dot{\tilde{\Phi}}_k|^2 + |\Phi_k|^2 \dot{\phi}^2) + \frac{E_J}{2} |\tilde{\Phi}_k|^2. \tag{3.32}$$

Note that we left out the geometric phase here. We will take that into account again later. We have seen that it does not change the instanton solution in sec. 3.2. Then we derive the equation of motion for the complex phase $\tilde{\Phi}_k$

$$\Rightarrow |\tilde{\Phi}_k|^2 \ddot{\phi}_k = 0, \tag{3.33}$$

which is always fulfilled when $|\Phi_k| = 0$, where it loses its meaning, and afterwards it only says that there is no acceleration. Since we want the instanton solution to approach a certain value, the complex phase then has to be fixed. Since this does not depend on any parameter of the system and this motion of the complex phase does not give any contribution to the action, we can neglect that and just focus our attention on the absolute values of the variables

$$\frac{\hbar^2}{8E_C}(1-\eta\cos(2\pi\frac{k}{N}))|\ddot{\tilde{\Phi}}_k| = E_J|\tilde{\Phi}_k|. \tag{3.34}$$

We can solve this for $-\infty < t < 0$ and therefore also get the solution for $0 < t < \infty$. With $|\tilde{\Phi}_k^{Final}|$ as the values, that the instanton solution approaches for $t \to \infty$, we get

$$\Rightarrow |\tilde{\Phi}_k(t)| = \begin{cases} |\tilde{\Phi}_k^{Final}|\frac{1}{2}e^{\sqrt{\frac{8E_JE_C}{\hbar^2(1-\eta\cos(2\pi\frac{k}{N}))}}t} & t<0 \\ |\tilde{\Phi}_k^{Final}|(1-\frac{1}{2}e^{-\sqrt{\frac{8E_JE_C}{\hbar^2(1-\eta\cos(2\pi\frac{k}{N}))}}t}) & t>0 \end{cases}. \tag{3.35}$$

In order to use that, we have to find $|\tilde{\Phi}_k^{Final}|$. For the instanton defined above, where the islands from $r+1$ to $M+r$ tunnel we get

$$\tilde{\Phi}_k^{Final} = \frac{2\pi}{\sqrt{N}}\sum_{j=1}^{M} e^{2\pi i\frac{k}{N}(r+j)} = \frac{2\pi}{\sqrt{N}}e^{2\pi i\frac{k}{N}(r+1)}\frac{1-e^{2\pi i\frac{k}{N}M}}{1-e^{2\pi i\frac{k}{N}}} \tag{3.36}$$

$$\Rightarrow |\tilde{\Phi}_k^{Final}|^2 = \frac{4\pi^2}{N}\frac{\sin^2(\pi\frac{k}{N}m)}{\sin^2(\pi\frac{k}{N})}. \tag{3.37}$$

Now we can calculate the action corresponding to the instanton solution. Since the different variables are uncoupled, the action of the whole path splits into contributions from the paths of the single variables, that can be calculated like in the single Island case, therefore

$$S_M = \sqrt{\frac{E_J}{8E_C}}\frac{\pi^2}{N}\sum_{k=1}^{N}\sqrt{1-\eta\cos\left(2\pi\frac{k}{N}\right)}\frac{\sin^2(\pi\frac{k}{N}M)}{\sin^2(\pi\frac{k}{N})}. \tag{3.38}$$

We can see that the contribution from long wave length, i.e, for k close to one or k close to N, are very small for large η, because of the factor $\sqrt{1-\eta\cos\left(2\pi\frac{k}{N}\right)}$. In the instanton solution Eq. (3.35) we can see that those modes move quickly compared to other modes. This can be used to argue why the Villain approximation should be good in the large η limit. Let us think about an example instanton where $N/2$ neighboring islands tunnel, therefore $|\tilde{\Phi}_0^{Final}| \approx \pi$. Since the $k = 0$ variable is arbitrarily fast in the $\eta \to 1$ limit, we can treat that movement as instantaneous compared to all other movements. Therefore the instanton solution has to jump from

$$\Phi_j(0^-) = \begin{cases} \Phi_j = \frac{\pi}{2} & r+1 \le j \le r+\frac{N}{2} \\ \Phi_j = -\frac{\pi}{2} & \text{else} \end{cases} \tag{3.39}$$

to

$$\Phi_j(0^+) = \begin{cases} \Phi_j = \frac{3\pi}{2} & r+1 \leq j \leq r+\frac{N}{2} \\ \Phi_j = \frac{\pi}{2} & \text{else} \end{cases}. \tag{3.40}$$

The jump itself, i.e, the zero mode does not contribute to the action in the $\eta \to 1$ case. The important observation to make in this example is that the complete motion, that contributes to the action, keeps all islands in a range where the Villain approximation is very good, namely $-\pi/2 < \Phi_j < \pi/2$. Now one might argue, that we are not only interested in instantons where $N/2$ islands tunnel. Especially when we let N go to infinity later, that case itself is not interesting. The idea that the two islands at the border of the tunneling cluster move to $\Phi_r = -\pi/2$ and $\Phi_r + 1 = \pi/2$ and then the long wavelength modes move the cluster through the higher potential very quickly and without picking up much action should be generalizable though, because the movement at the border of the tunneling cluster has to be dominated by modes with short wavelength, which dominate the dynamics far away from $t = 0$. Close to $t = 0$ the modes with long wavelength move very abruptly again and do not pick up very much action because of that. Therefore we do not expect the part of the potential, where the Villain approximation is bad to change the action of the instanton very much. But we will do numerics to test that.
Now we want to evaluate the sum in the expression of the action of the different instantons. We have to do that to get an explicit interaction between the charge offsets in terms of a power law or exponential decay later. Since we are interested in large systems $N \to \infty$ we can interpret the sum as a Riemann sum and write it as an integral

$$S_M = \sqrt{\frac{E_J}{8E_C}}\pi \int_0^\pi \sqrt{1-\eta\cos(2k)}\frac{\sin^2(kM)}{\sin^2(k)}dk. \tag{3.41}$$

This enables us to use contour integration methods to evaluate this sum. For that we will change the form of the integrand, so that it decreases rapidly for large imaginary parts of k. Of course we leave the function unchanged on the real domain. So we choose the form

$$S_M = \sqrt{\frac{E_J}{8E_C}}\pi \int_0^\pi \sqrt{1-\eta\cos(2k)}\frac{\mathrm{Re}(1-e^{2ikM})}{2\sin^2(k)}dk. \tag{3.42}$$

Now we want to commute the integral with taking the real part, but have to take care, because that does not commute trivially. By not taking the real part in the integrand we change the discontinuities at $k = 0$ and $k = \pi$ from a removable to an infinite discontinuity. We are going to account for that by subtracting terms with the same behavior in those two points, but that are holomorphic everywhere else

$$S_M = \sqrt{\frac{E_J}{8E_C}}\pi\mathrm{Re}\int_0^\pi \sqrt{1-\eta\cos(2k)}\frac{1-e^{2ikM}}{2\sin^2(k)} + \frac{iM\sqrt{1-\eta}}{k} + \frac{-iM\sqrt{1-\eta}}{(k-\pi)}dk. \tag{3.43}$$

Now we can split the integral in a sum of integrals to choose individual integration contours for the different contributions of the integrand. Let us

start with the correction terms, since they are rather simple. We are going to choose the integration paths $k = 0 \to i\pi \to \pi$ for the first and analog to that $k = 0 \to (1+i)\pi \to \pi$ for the second correction term. We will only look at the first integral explicitly, because the second one can be done analogously. Since we are only looking at real contributions those integrals come down to a quarter residuum each, because

$$\mathrm{Re}\left(\int_0^{i\pi} \frac{iM\sqrt{1-\eta}}{k} dk\right) = 0. \tag{3.44}$$

That integral would be completely imaginary, therefore the real part is zero. So that only leaves

$$\mathrm{Re}\left(\int_{i\pi}^{\pi} \frac{iM\sqrt{1-\eta}}{k} dk\right) = \frac{\pi M\sqrt{1-\eta}}{2}. \tag{3.45}$$

The second correction term yields the same result, so that their combined contribution is $\pi M\sqrt{1-\eta}$. That leaves the original part of the integral. Here we choose the integration path $k = 0 \to i\infty \to i\infty + \pi \to \pi$. We know

$$\mathrm{Re}\int_{i\infty}^{i\infty+\pi} \sqrt{1-\eta\cos(2k)}\frac{1-e^{2ikM}}{2\sin^2(k)} dk = 0, \tag{3.46}$$

because the integrand converges to zero for $\mathrm{Im}(k) \to \infty$. Now we are left with two contributions

$$\mathrm{Re}\int_0^{i\infty} \sqrt{1-\eta\cos(2k)}\frac{1-e^{2ikM}}{2\sin^2(k)} dk$$

and

$$\mathrm{Re}\int_{i\infty+\pi}^{\pi} \sqrt{1-\eta\cos(2k)}\frac{1-e^{2ikM}}{2\sin^2(k)} dk.$$

It is important to note, that those terms do not cancel, as one might think due to the integrand, that seems to be π-periodic. But if we avoid putting the branchcut of the square root in the integration path, to avoid correction terms for the change of the integration path, we see that the integrals contribute equally. Therefore it is enough to calculate one of the integrals. So let us take a look at the first one

$$\mathrm{Re}\int_0^{i\infty} \sqrt{1-\eta\arccos(2k)}\frac{1-e^{2ikM}}{2\sin^2(k)} dk = \int_{\frac{1}{2}\mathrm{acosh}(\eta^{-1})}^{\infty} \sqrt{\eta\cosh(2k)-1}\frac{1-e^{-2kM}}{2\sinh^2(k)} dk. \tag{3.47}$$

Here we changed the integration variable by a factor of i and reduced the integration range to the area that gives a real contribution. Solving this integral exactly is not simple, but we can make a distinction between two solvable approximations. If $M \gg \frac{1}{\mathrm{acosh}(\eta^{-1})} \approx \sqrt{\frac{\eta}{2(1-\eta)}}$, then e^{-2kM} is very small over the whole integration range, and can therefore be neglected. That makes the integral independent of M. The only parameter left in there is η. Rather than

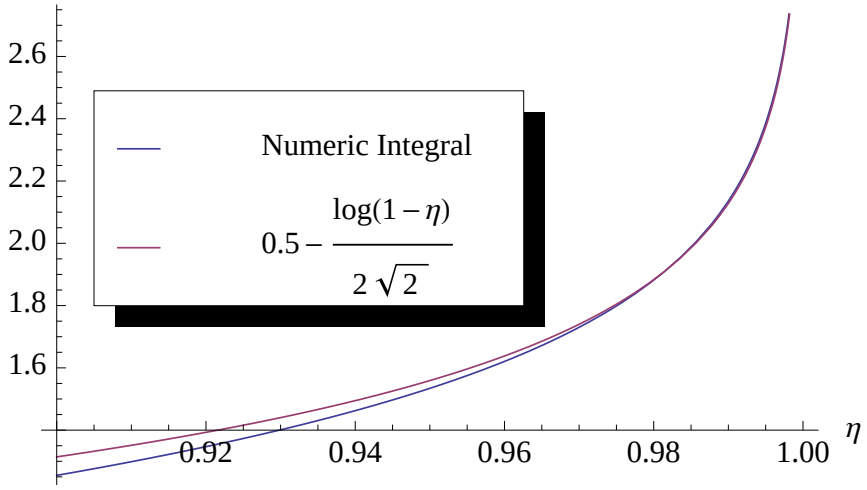

Figure 3.6: For $M \gg \sqrt{\frac{2\eta}{(1-\eta)}}$ both sides of Eq. (3.48) are plotted, where the integral was evaluated numerically. Especially the scaling for $\eta \to 1$ is correct.

putting much effort into this integral we can do that integral numerically and show how it scales for large η. Fig. 3.6 shows

$$\int_{\frac{1}{2}\mathrm{acosh}(\eta^{-1})}^{\infty} \frac{\sqrt{\eta\cosh(2k)-1}}{2\sinh^2(k)}dk \approx -\log(1-\eta)/\sqrt{8}+0.5. \tag{3.48}$$

Now that we have found the scaling for large M, we also need to find the behavior for $M \ll \frac{1}{\mathrm{acosh}(\eta^{-1})}$. Note that this is only possible for very large η, because otherwise we would require $M < 1$, which means no tunneling at all. This time the idea is to approximate $1-e^{-2kM}$ as a theta function moving the lower integration boundary to $\frac{1}{2M}$. In this region of the integral $\sqrt{\eta\cosh(2k)-1}$ is dominated by the $\cosh(2k)$ term. Hence

$$\begin{aligned} &\int_{\frac{1}{2}\mathrm{acosh}(\eta^{-1})}^{\infty} \sqrt{1-\eta\cosh(2k)}\frac{(1-e^{-2kM})}{2\sinh^2(k)}dk \\ \approx &\int_{\frac{1}{2M}}^{\infty} \sqrt{\frac{\eta}{2}}\frac{1}{\sinh(k)}dk \approx \sqrt{\frac{\eta}{2}}(\log(4M)+\gamma)+O\left(\frac{M}{\mathrm{acosh}(\eta^{-1})}\right), \end{aligned} \tag{3.49}$$

where γ is Euler's constant $\gamma \approx 0.577$. This approximation was checked numerically in Fig. 3.7. Putting all those results together and taking the prefactor into account again we get

$$S_M \approx \begin{cases} \sqrt{\frac{\eta E_J}{4E_C}}\pi\log(4M)+\sqrt{\frac{\eta E_J}{4E_C}}\pi\gamma+\sqrt{\frac{E_J}{8E_C}}\pi^2 M\sqrt{1-\eta}, M \ll \sqrt{\frac{2\eta}{1-\eta}} \\ \sqrt{\frac{E_J}{8E_C}}\pi^2 M\sqrt{1-\eta}-\sqrt{\frac{E_J}{64E_C}}\pi(\log(1-\eta)-\sqrt{2}), \quad M \gg \sqrt{\frac{2\eta}{1-\eta}} \end{cases}. \tag{3.50}$$

This equation yields the interaction in the system, as will be shown in the following. To understand that, we have to make a dilute gas approximation again.

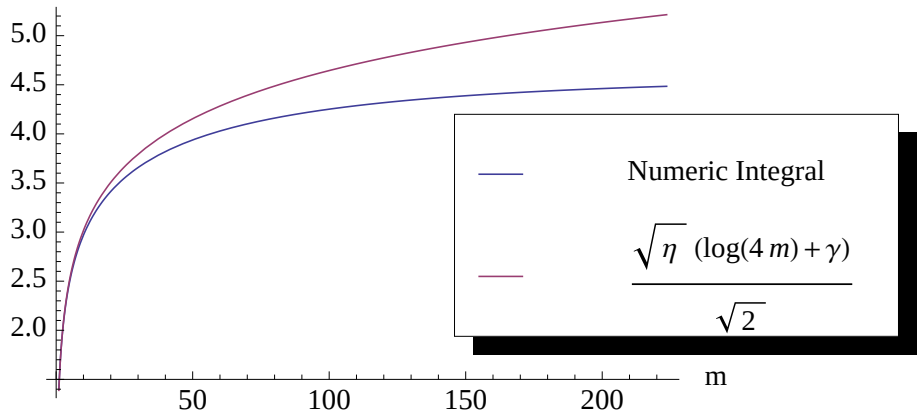

Figure 3.7: Here we plotted the numerical result of the integral and the right side of Eq. (3.49) for $M \ll \sqrt{\frac{2\eta}{(1-\eta)}}$ at $\eta = 0.9999$.

There we approximate all tunneling solutions between potential minima. In the calculation for a single Cooper pair box, we have seen, that we can approximate multi tunneling events as a series of single tunneling events. In the multi box system one might then argue, that we do not need instanton solutions with more than one island tunneling, because we could approximate many islands tunneling by a series of single island tunneling events. But since the action is not linear in M for simultaneous tunneling at $\eta \neq 0$, this approximation would brake down in this case and underestimate the tunneling rate. Especially since we have seen that single tunneling events only depend on one charge, we would loose all charge interactions with that approximation. Therefore we have to take those events into account separately. Now one might wonder why we only considered M neighboring islands tunneling simultaneously in one direction. There could also be two separated tunneling clusters, or two neighboring tunneling clusters tunneling in opposite directions, or other constructions. We assume, that the dilute gas approximation will work for those cases, if we only take single tunneling clusters into account. The argument for that was already established earlier. We understood, that the action is mainly caused by the requirement for neighboring islands to tunnel with respect to each other. Therefore the action of separated tunneling clusters tunneling simultaneously should be well approximated by the sum of the actions of each cluster tunneling by itself. In the case of neighboring clusters tunneling in opposite directions, the action might even be underestimated, because the zero mode cannot be used to tunnel two clusters in opposite directions at once. But the dilute gas approximation is not very sensitive to that, because as discussed before, the integral over all time configurations is already dominated by well separated instantons. So making instantons coming closer to each other even less probable should not change the result much. Only when simultaneous events become much more probable, that has to be taken into account. Note that the question whether a certain event has to be taken into account separately is similar to

the question whether a diagram in diagrammatic perturbation theory is irreducible. There one argues whether we can build a complex diagram from a set of simpler ones. In the instanton calculation we argued whether certain more complex instantons could be approximated by a set of simpler ones. In that sense these tunneling clusters of arbitrary size are irreducible tunneling events. Let us now take a more explicit look at the dilute gas calculation. We get an integral over all time configurations, a sum over the number of tunneling events m and m sums over all irreducible tunneling events again. We also get a sum over all positions r of the tunneling cluster of a certain size M. The factors F_M are analogous to the factor F in Eq. (3.22) and Θ_{geo} are the geometric phases picked up by the instanton

$$\langle \mathbf{0}|e^{iHT/\hbar}|\mathbf{0}\rangle \propto \sum_{m=0}^{\infty} \int dt_1 ... dt_m \left(\sum_r \sum_M F_M e^{-S_M} \cos(\Theta_{geo}(M,r)) \right)^m , \quad (3.51)$$

with

$$\Theta_{geo}(M,r) = \sum_{j=r+1}^{r+M} \frac{\pi q_j}{e} \quad (3.52)$$

In the last section we only had two irreducible tunneling events, namely tunneling up and tunneling down. The opposite geometric phases resulted in the Aharonov-Casher effect. This time we have more irreducible tunneling events, that pick up different geometric phases. There still is the Aharonov-Casher effect, because each tunneling cluster can tunnel either up or down. The groundstate energy corrections are

$$\Delta E(\boldsymbol{q}) = \sum_r \sum_M F_M e^{-S_M} \cos(\Theta_{geo}(M,r)). \quad (3.53)$$

The geometric phases depend on the sum of the charge offsets of all tunneling islands. Since we are interested in two point interactions let us assume only two islands with distance d, where $d = 1$ for neighboring islands, have charge offsets with $q_j \neq 0$. Let those islands be at position $r+1$ and $r+d+1$. Then for the interaction terms we only need to look at those instantons where both those islands tunnel, because otherwise the groundstate energy correction depends only on one charge. Let us assume for now, that the sum is dominated by the term with minimal M. This minimal value is $M = d+1$ because if the distance between two islands is d, a tunneling cluster including both those islands has at least $d+1$ islands. So we get interactive groundstate energy corrections

$$\Delta E_d \cos\left(\frac{(q_{r+1} + q_{r+d+1})\pi}{e} \right), \quad (3.54)$$

with

$$\Delta E_d = 4F_{d+1}e^{-S_M}$$
$$= 4F_{d+1}e^{-\sqrt{\frac{E_J(1-\eta)}{8E_C}}\pi^2(d+1)} \begin{cases} (4(d+1))^{-\pi\sqrt{\frac{\eta E_J}{4E_C}}} e^{-\sqrt{\frac{\eta E_J}{8E_C}}\gamma} & d+1 < \sqrt{\frac{2\eta}{1-\eta}} \\ e^{-\sqrt{\frac{E_J}{32E_C}}\pi} (1-\eta)^{-\sqrt{\frac{E_J}{64E_C}}\pi} & d+1 > \sqrt{\frac{2\eta}{1-\eta}}. \end{cases} \quad (3.55)$$

Here we can see how the interaction strength scales with d, except for the prefactor F_M. The problem is, that the Gelfand-Yaglom equation only works for one dimensional differential operators. So we can not calculate those prefactors. If we assume them not to decrease exponentially with M then in the $\eta \to 1$ limit, we get a power law with diverging range, and a vanishing screening. It is also interesting, that the power law can be tuned by the parameter $\frac{E_J}{E_C}$. Note that this power grows with larger $\frac{E_J}{E_C}$. One should have expected that because the more the local potential energy dominates the physics of the system, the less we can expect strong correlations between different islands.
Now let us briefly discuss what happens in systems, where the action rises slowly, so that the the sum in Eq. (3.53) is not dominated by one term. Then we have to evaluate the sum $\sum_{M=d+1}^{\infty}(M-d)e^{-S_M}$, to get ΔE_d. Note the factor $M-d$, because larger clusters have more possible positions, to include both charge offsets. If e^{-S_M} changes slowly with M, we can approximate

$$\sum_{M=d+1}^{\infty}(M-d)e^{-S_M} \sim \int_{d-\frac{1}{2}}^{\infty}(M-d)e^{-S_M}dM. \tag{3.56}$$

The important point here is, that in a region where e^{-S_M} scales like a mononom in M, the integral should still scale like a mononom and not exponentially. Therefore it is enough to look at that first term in the sum of Eq. (3.53), in order to see whether we have a long range interaction. Since we cannot find the exact potential, due to the missing prefactors, the remaining terms of that sum can be left out. Without further discussion we also assume that integral to decay exponentially in a region where e^{-S_M} decays exponentially. So we expect the screened interaction to stay screened as well.

3.4 Numerical Instanton Solution

In this section we will briefly discuss the basic idea of a program designed to find instanton solutions and their corresponding action. Afterwards we will compare its results for our problem of capacitively coupled Cooper pair boxes with the analytic result.
In the system of coupled Cooper pair boxes the quasi classical equation of motion is a second order differential equation. Usually in classical physics one solves such an equation with given position and velocity at one point of time. With those boundary conditions we could set up numerics, that use the equation of motion to develop the position and velocity in time. In the instanton calculation we have different boundary conditions though. We have the start and end point of that path. Therefore solving for the instanton using the equation of motion is problematic. In the analytic case we were able to do that because we approximated the system as many one dimensional, non interacting subsystems. We were able to use energy conservation in each of them to find the instanton solution. In the interacting case we have less known conserved quantities, therefore we cannot find the instanton solution as easily here. Rather than using the equation of motion, which is derived as a requirement for the

path with minimized action, we will directly minimize the action. That is also helpful to address the problem, that an instanton solution only approaches the start and end point. In the numerical calculation, an infinite time interval could not be handled. Even though we cannot use energy conservation in many dimensions to get an expression of the action without an explicit dependence on the instanton path, we can use energy conservation to reparameterize the path. Such a new timescale can squeeze the instanton on a finite domain. Let us do that step by step. We have an action of the form

$$S[\mathbf{\Phi}(t)] = \int_{-\infty}^{\infty} \dot{\mathbf{\Phi}}^T(t) T_{kin} \dot{\mathbf{\Phi}}(t) + V\left(\mathbf{\Phi}(t)\right) dt, \tag{3.57}$$

where S is the action, $\mathbf{\Phi}(t)$ represents all phases again, T_{kin} is a matrix with which we calculate the kinetic energy and V is the potential energy. Note that we are assuming a quadratic dispersion relation here. On classical paths, which the instanton solution has to be, we can then use energy conservation to get

$$S[\mathbf{\Phi}(t)] = \int_{-\infty}^{\infty} 2V\left(\mathbf{\Phi}(t)\right) dt \tag{3.58}$$

and for any parameterization $\lambda(t)$ with $\dot{\lambda}(t) \geq 0$

$$\frac{dt}{d\lambda} = \sqrt{\frac{\mathbf{\Phi}'^T(\lambda) T_{kin} \mathbf{\Phi}'(\lambda)}{V(\mathbf{\Phi}(\lambda))}}, \tag{3.59}$$

where $\mathbf{\Phi}'(\lambda)$ is the derivative of $\mathbf{\Phi}$ with respect to λ. Therefore we can change the integration variable in the expression of the action and get

$$S[\mathbf{\Phi}(\lambda)] = \int_{\lambda(-\infty)}^{\lambda(\infty)} 2\sqrt{\mathbf{\Phi}'^T(\lambda) T_{kin} \mathbf{\Phi}'(\lambda) V(\mathbf{\Phi}(\lambda))} d\lambda, \tag{3.60}$$

which is independent of the explicit dependence of λ on t. Therefore we can just choose $\lambda(-\infty) = 0$ and $\lambda(\infty) = 2\pi$, and go on with the calculation without choosing an explicit $\lambda(t)$. In order to find the instanton solution we are going to minimize the action. To do that we start out with any path with the required boundary conditions and set up a space of variations. Then we express the action as a function of the amplitudes of those variations and use an optimization routine to minimize that. Of course we can only choose a finite dimensional space of variations, to be able to implement this. The question, whether we took enough and the right variations into account will be the main uncertainty concerning the results of that calculation. In our program we used Fourier modes as variations. The idea here is, that all infinitely many modes would be a complete basis on the space of variations, but the kinetic energy term $\sqrt{\mathbf{\Phi}'^T(\lambda) T_{kin} \mathbf{\Phi}'(\lambda)}$ prefers smooth paths, i.e, the low modes. Therefore a finite number of modes should be enough to find the stationary path in a good approximation. In the program we increase that number of variations, until the minimized action does not change much anymore. The problem here is, that we do not know a convergence criterion, that ensures that the action is definitely

close to completely converged. We have just tried to make the convergence criterion rather strict, in the sense that the action does not change much when we add more than one additional Fourier mode. Note that Eq. (3.59) implies that the new parameterization helps to keep the number of required Fourier modes low, because the time is less squeezed at high energies, where the movement is fast and therefore would require high modes. In the analytic calculation we took the limit of infinitely many islands. In the numerical calculation that is not possible. Therefore we treated the number of islands similarly to the number of variations. We increased the number of islands, until the action seemed to be converged.

Now that we understand the basic idea of how the numerical results were achieved, we can compare them to the analytic results and discuss that. In Fig. 3.8 we can see a good agreement between the numerical and analytic results changed by a prefactor. In the many island calculation of the instanton action with the Villain approximation we had prefactors $\pi^2/\sqrt{8}$. We changed them to $\sqrt{8}$. The idea here is that those prefactors are the exact actions we get in a single Cooper-pair box for tunneling events with and without the Villain approximation. So the plotted analytic action is

$$S_M \approx \begin{cases} \sqrt{\frac{16\eta E_J}{\pi^2 E_C}}\log(4M) + \sqrt{\frac{16\eta E_J}{\pi^2 E_C}}\gamma + \sqrt{\frac{8E_J}{E_C}}M\sqrt{1-\eta}, M \ll \sqrt{\frac{2\eta}{1-\eta}} \\ \sqrt{\frac{8E_J}{E_C}}M\sqrt{1-\eta} - \sqrt{\frac{E_J}{\pi^2 E_C}}(\log(1-\eta)-\sqrt{2}), \qquad M \gg \sqrt{\frac{2\eta}{1-\eta}} \end{cases} . \tag{3.61}$$

Note that it takes long calculation times to get solutions for high η, therefore it is difficult to simulate systems with very long ranged interactions. Also that the agreement in Fig. 3.9 is limited by the approximation tested in Fig. 3.7.

Since we cannot prove that the numerics are completely converged one might argue, that the numerics cannot be trusted and that therefore we should trust the formula derived analytically without any changes of prefactors. But since the action found in the numerical calculation is lower than the analytic action, the numerical path has to be closer to the optimal path than the one from the analytic calculation. But the important fact is the qualitative agreement anyway. Therefore we can still assume, that the analytic calculation captures the important mechanisms in the system. Especially since both results show the tendency to long ranged interactions for large η, which is the main result.

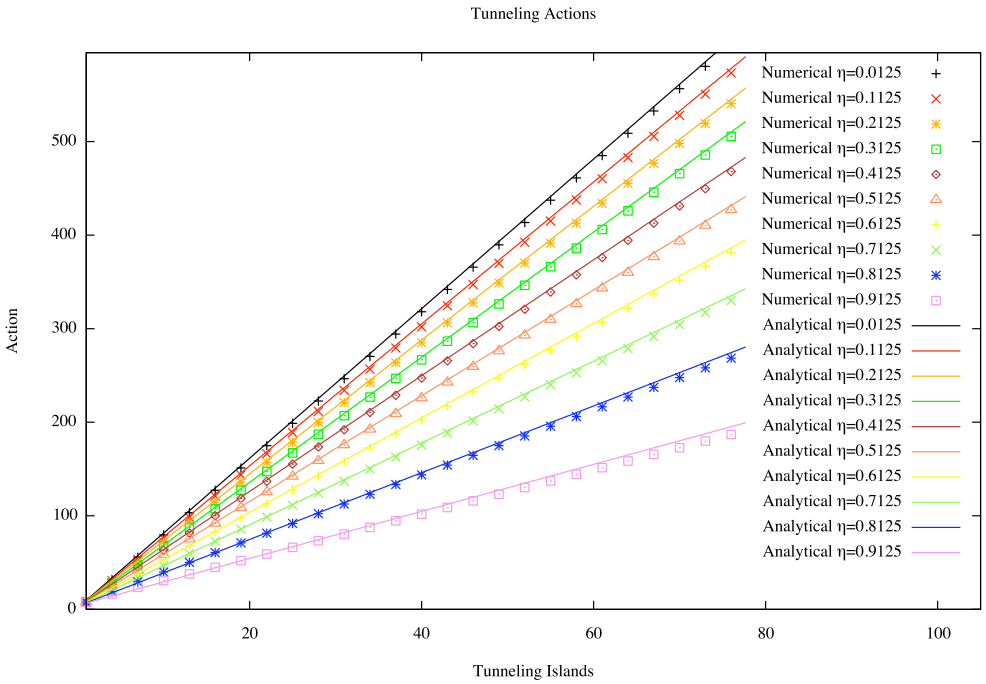

Figure 3.8: Here we can see plots of numerically calculated actions compared to analytically calculated actions for many islands tunneling, only changed by a prefactor. For all graphs here we set $\frac{E_J}{E_C} = 8$.

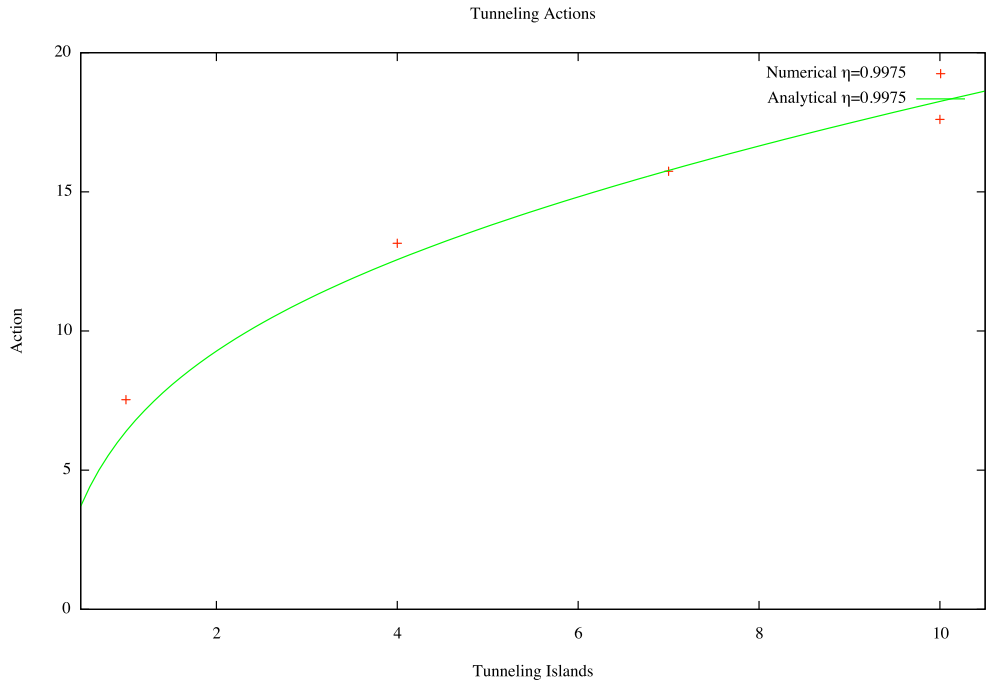

Figure 3.9: Here we see a plot of numerically calculated actions compared to analytically calculated actions for only a few islands tunneling, again changed by a prefactor. We set $\frac{E_J}{E_C} = 8$.

Chapter 4

Ground state approximation

In this chapter we are going to construct an effective low energy Hamiltonian for the Cooper pair box and find a way to get the ground state energy from first order perturbation theory in the ground state of that low energy Hamiltonian. We will then show, that the ground state of a Cooper pair box with a Villain approximation of the potential is well approximated by a single basis state of the low energy Hamiltonian. With that knowledge we approximate the ground state of the many island system. In the end we will compare the results of that approximation with the results from the path integral formalism.

4.1 Single Cooper pair box

In order to construct an effective low energy Hamiltonian let us take a look at the Hamiltonian of a single Cooper-pair box again

$$H = 4E_C(i\partial_\Phi - \frac{q}{2e})(i\partial_\Phi - \frac{q}{2e}) + E_J(1 - \cos(\Phi)). \tag{4.1}$$

The charge offsets can again be gauged away as in chapter 2. Since we assume $E_J \gg E_C$ the low energy eigenstates should be very similar to harmonic oscillator eigenstates, because we expect them to be well localized in the parabolic part of the potential. Therefore we use harmonic oscillator energy eigenstates to construct a basis for the low energy Hamiltonian. Since we have a 2π-periodic potential we are also going to make the basis states periodic, by adding harmonic oscillator eigenfunction localized in each well of the potential. So let us construct those states explicitly. If $H_m(\Phi)$ is the m-th harmonic oscillator eigenfunction, then we choose our basis states $\Psi_m(\Phi)$

$$\Psi_m(\Phi) = \sum_{n=-\infty}^{\infty} e^{-i(\Phi+2\pi n)q} H_m(\Phi + 2\pi n). \tag{4.2}$$

Note that we Φ only goes from 0 to 2π. The periodicity condition can be understood by thinking of the domain as a ring. To get a low energy Hamiltonian we are going to take the M lowest states into account. Since the basis states should be close to the eigenstates we do not need to use more complicated techniques than that. We can then develop the Hamiltonian in a $M \times M$ matrix. Note that

those states are not necessarily orthogonal, even though the harmonic oscillator states are. Because of that non orthonormal basis, we also need to calculate the overlap of the different basis states. Usually one puts that into a matrix S

$$S_{m,m'} = \int_{-\pi}^{\pi} \Psi_m(\Phi)\Psi_{m'}(\Phi)d\Phi. \tag{4.3}$$

To get the eigensystem of the problem we have to solve the generalized eigenvalue problem

$$H|\Psi\rangle = ES|\Psi\rangle. \tag{4.4}$$

The strength of that approach is, that we can numerically solve for the ground state at $q = 0$ and then do a first order perturbation theory in q and already get the whole perturbation proportional to $\cos(\pi q/e)$. To understand that we have to look at perturbation theory for non orthonormal basis states and into the calculation of matrix elements for that basis. Let us start with the first order perturbation of the energy eigenvalue

$$\Delta E = \frac{\langle\Psi|H_P|\Psi\rangle - E\langle\Psi|S_P|\Psi\rangle}{\langle\Psi|S|\Psi\rangle}. \tag{4.5}$$

Where H_P and S_P are the changes in H and S due to the change of q. Let us now take a look at the calculation of matrix elements of a linear operator in the basis discussed above. Remember, that we used a gauge transformation on that basis, to gauge the charge offsets away. Therefore we get

$$O_{m,m'} = \int_{-\pi}^{\pi} \Psi_m(\Phi)O\Psi_{m'}(\Phi)d\Phi \tag{4.6}$$

$$\Rightarrow O_{m,m'} = \sum_{n,n'=-\infty}^{\infty} e^{i2\pi(n'-n)} \int_{-\pi}^{\pi} H_m(\Phi + 2\pi n)OH_{m'}(\Phi + 2\pi n')d\Phi. \tag{4.7}$$

Let us assume the operator O to also be 2π periodic, because of the 2π periodicity of the phase Φ. Then a change of summation variables yields

$$\Rightarrow O_{m,m'}$$
$$= \int_{-\infty}^{\infty} H_m(\Phi + 2\pi n)OH_{m'}(\Phi)d\Phi + \sum_{n=1}^{\infty}(e^{2\pi qn} \pm e^{-2\pi qn}) \int_{-\infty}^{\infty} H_m(\Phi + 2\pi n)OH_{m'}(\Phi)d\Phi. \tag{4.8}$$

The $\pm$ depends on whether the state H_m and $H_{m'}$ are symmetric or antisymmetric. The ground state should be symmetric like the harmonic oscillator ground state, which is why we get a plus sign i.e. a $\cos(2\pi qn)$ when we do first order perturbation theory on the ground state energy. Since we assumed $E_J >> E_C$ the overlap of two low harmonic oscillator eigenstates should be small when their centers are further apart than 2π. Therefore we can approximate the sum over all offsets n as $\sum_{n=-1}^{1}$ rather than $\sum_{n=-\infty}^{\infty}$. Therefore the perturbation in q is already proportional to $1 - \cos(\pi q/e)$. We also expect higher orders of perturbation theory to be negligible, because of the small overlap of different

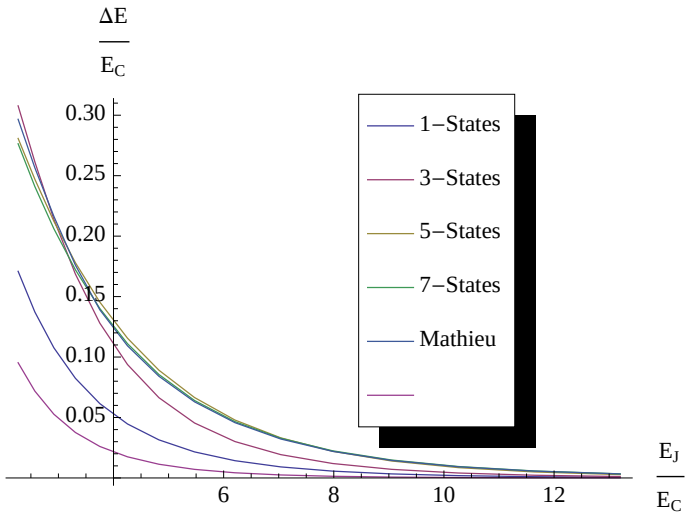

Figure 4.1: With enough states in the low energy Hamiltonian there is a similarity, but no exact agreement between this calculation and the known results.

harmonic oscillator eigenstates. As mentioned before the whole calculation can be done numerically. In Fig. 4.1 there are the results for calculations with a different number of states in the effective low energy Hamiltonian. Let us now look at the Cooper pair box with a Villain approximation on the potential in Φ, as introduced in the last chapter for the many island case. It is interesting to see, that in a Villain potential the approximation with $M = 1$ i.e. a direct ground state approximation through harmonic oscillator ground states works well. We can see that in figure 4.2, where the results depend very little on the number of states in the effective Hamiltonian. So we have found a ground state approximation in the Villain Potential. Let us use that for the many island system.

4.2 Coupled Cooper pair boxes

We will use the ground state approximation of the last section in the many island system, because if we wanted to take excited states into account there we would have the problem of the Hilbert space growing exponentially with the number of island. Note that we will have to use the Villain potential again, because otherwise the ground state approximation was not good enough to find the energy splitting due to offsets charges accurately. Before we do that, we will change the variables to get uncoupled harmonic oscillators again. Near one potential minimum the Hamiltonian without charge offsets can be approximated as

$$\Rightarrow H = \sum_{j=1}^{N}(\sum_{j'=1}^{N} 4E_C(C_M)^{-1}_{j,j'}Q_jQ_{j'} + \frac{E_J}{2}\Phi_j^2. \tag{4.9}$$

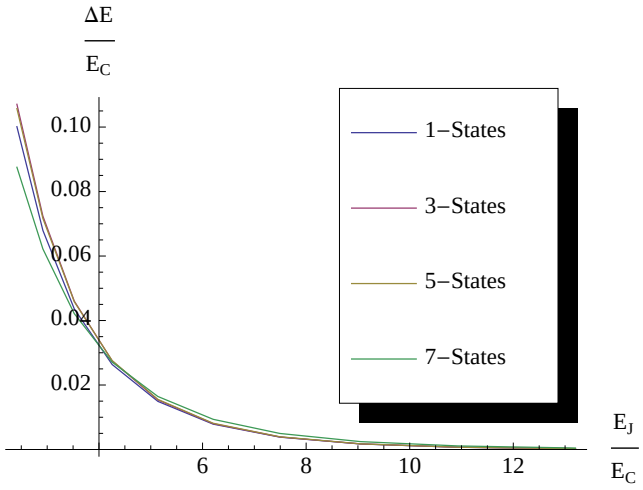

Figure 4.2: The direct convergence suggests, that the ground state was approximated well in the single state case.

A Fourier series gets rid of the interactions again. Note that $\tilde{Q}_k = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{2\pi i \frac{k}{N} j} Q_j$ is still the canonical conjugate to $\tilde{\Phi}_k$. Then the Hamiltonian looks like this

$$H = \sum_{k=1}^{N} -\frac{4E_C}{(1 - \eta \cos(2\pi \frac{k}{N}))} \partial^2_{\tilde{\Phi}_k} + \frac{E_J}{2} \tilde{\Phi}_k^2. \tag{4.10}$$

The harmonic oscillators are now in terms of the transformed variables, but there they are uncoupled, therefore we know the ground state. Just like in the single island case we have to sum over harmonic oscillator states in all potential minima, which was easily done by summing over one variable. In the many island case we have to take a sum over one variable per island to take all minima into account. All those variables are put together in a vector $\boldsymbol{n}$. Note that those vectors are offsets in the old variables Φ_j. In our state written in terms of $\tilde{\Phi}_k$ those vectors have to be transformed as well, which is indicated by $\tilde{\boldsymbol{n}}$ or its elements $\tilde{n}_k$.

$$\Psi(\tilde{\boldsymbol{\Phi}}) = \sum_{n_1, n_2, \ldots, n_N = -\infty}^{\infty} e^{-i(\Phi + 2\pi \boldsymbol{n})\boldsymbol{q}} e^{-\sum_{k=1}^{N} \sqrt{\frac{E_J}{32E_C}(1 - \eta \cos(2\pi \frac{k}{N}))}(\tilde{\Phi}_k + \tilde{n}_k)^2} \tag{4.11}$$

We were able to drop all normalization factors, since we do not rely on an orthonormal system anyway. With that state we can do exactly the same perturbation theory as before. In the single island case we approximated the sum over all offsets as $\sum_{n=-1}^{n}$. In the many island case we are going to sum over the vectors $\boldsymbol{n} = \boldsymbol{0}$ and the vector with an offset for both boxes with charge offset and the boxes in between in both directions. That means if we have charge offsets on box 1 and box $d+1$, then the offset vectors we take into account are $\boldsymbol{n} = \boldsymbol{0}$, $\boldsymbol{n} = \sum_{j=1}^{d+1} \boldsymbol{e}_j$ and $\boldsymbol{n} = -\sum_{j=1}^{d+1} \boldsymbol{e}_j$, which is analogous to the tunneling event we took into account in the path integral formalism. This choice was not apparent to us from the beginning, but it shows good agreement with the

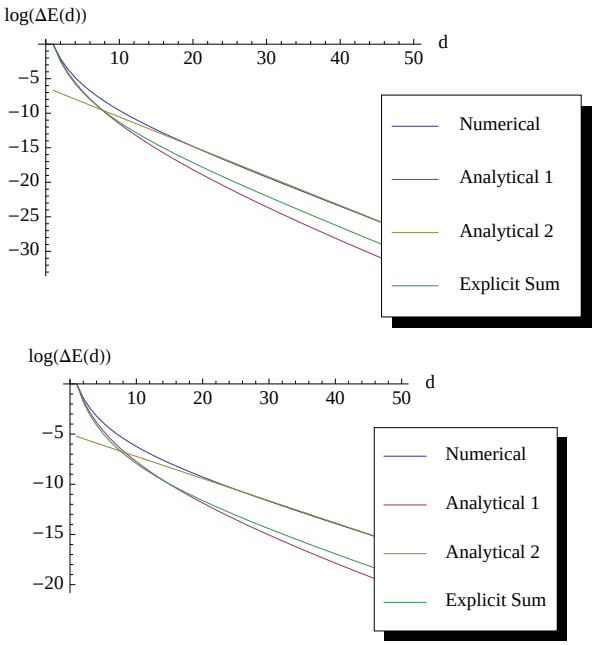

Figure 4.3: The system has 200 islands and periodic boundary conditions. In order to exclude effects, that are due to the periodicity of the system we only look at distance of up to 50 islands. The parameters are $\frac{E_J}{E_C} = 15$ and $\eta = 0.999$ in the first, and $\frac{E_J}{E_C} = 8$ and $\eta = 0.9995$ in the second graph. We compare the scaling of the interaction with the distance, therefore the single graphs were moved up/down, to be able to compare. Since we have a logarithmic plot, that does not change the scaling. We compare to the analytic short and long range behavior, as well as the exact sum from Eq. (3.38).

results from the path integral formalism, as can bee seen in Fig. 4.3. We do not know whether there is something analogous to the linked cluster theorem in the path integral formalism to explain that choice of offset vectors. We can see a good agreement between both calculations. Therefore our assumption that we can just ignore that quotient of determinants in the path integral formalism is supported by this calculation. Since this calculation has the weakness, that we do not have a strong argument for our choice of offset vectors we cannot be sure of that yet.

Chapter 5

Discussion and Outlook

We have understood the charging energy of a Cooper box via phase slips and an interference effect, the Aharonov-Casher effect. In order to generalize that we have found instanton solutions for phase slips in the many island system. There it turned out, that neighboring islands tunneling simultaneously induce charging energy depending on more than one charge, i.e, interactions. The qualitative agreement between numeric and analytic results suggest that we understood these instanton solutions. Their action as a function of the number of tunneling islands suggests longrange interactions in the $\eta \to 1$ limit. The problem here is, that we cannot evaluate the integral over all variations around those instantons. We assume that this integral might change the form of the resulting interaction, but does not screen the interaction. In order to support this assumption we found a groundstate approximation for the system and used perturbation theory, with the offset charges as perturbations, to find the interactions in the system via a different calculation. The problem here was that the numerical calculation we made here would not have been effecient, if we had not assumed that analogy to the linked cluster theorem. Therefore those results cannot be trusted without further investigation. The similar scaling of the interactions resulting from both methods strongly point towards tunable long range interactions. If we want to use the system to simulate a long range Ising model, it would be very interesting to find the exact form and strength of the interaction, because otherwise we would only know, that we are simulating some long range Ising model, but not which. In order to do that in the path integral formalism we would have to find a way to do the integral over all variations in an interacting many dimensional system.

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