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Control of Quantum Evolution and Josephson Junction Circuits

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VTT Information Technology

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Abstract

Ever since Peter Shor's ground-breaking discovery in 1994 of an algorithm capable of factoring large integers on a quantum-mechanical computer exponentially faster than using any known classical method, research on quantum computing has boomed. Quantum information – a unique mixture of computer science, physics and mathematics – has developed into a new branch of information theory. On the experimental side, physicists from many different disciplines including atomic, solid-state and low-temperature physics, as well as optics, are striving today towards a practical quantum computer. All the candidate quantum bit (qubit) technologies have one thing in common: They rely on the controlled time-evolution of a closed quantum system, a seemingly paradoxical task.

In this Thesis the temporal control of quantum systems is studied. The topics included can be divided into two according to the type of temporal evolution; geometrical or dynamical. Geometrical realization-independent methods for quantum computing are studied first. Then the study is extended into dynamical quantum computing and the so-called Josephson charge-qubit register is considered as a test bench. Finally, a spin-off application of the geometrical evolution of a Josephson junction system is studied, i.e. Cooper pair pumping. A novel Cooper pair pump, the Cooper pair "sluice", is introduced.

The work on quantum computing reported in this Thesis is theoretical while the Cooper pair "sluice" is studied both theoretically and experimentally. Numerical simulations, both sequential and parallel, are used extensively throughout the Thesis. The experiments were carried out under cryogenic mK conditions and the sample fabrication was done using e-beam nanolithography.

Because the execution time of a quantum algorithm is always limited by the inevitable process of decoherence, it is important to utilize any measure available for accelerating quantum computations. It is found that practical quantum algorithms could greatly benefit from classical computer-aided optimization. Moreover, it is found that even a modest demonstrator of a full quantum algorithm using Josephson charge qubits is just barely realizable within present-day coherence times. However, the experimental part of this Thesis shows clear evidence of the functioning of the "sluice". While the worldwide effort of improving the coherence properties of qubits is underway, the "sluice" could well find practical use, e.g., in metrology in the foreseeable future.

Preface

The incentive for this work was obtained when I attended prof. Mikio Nakahara's course *Quantum Computing* in 2001 at Helsinki University of Technology (HUT) while he was in Finland as a visiting professor from Kinki University, Osaka. Later, in 2002, I had the privilege of writing my Master's Thesis under prof. Nakahara's guidance at the Materials Physics Laboratory of HUT. The Master's Thesis titled *Holonomic Quantum Computing*, lead to the first two papers of this Thesis. The next three papers of the work were on a slightly different subject, but still, they were a natural continuation of my Master's Thesis. I am grateful to prof. Nakahara for his guidance. I also wish to thank my Finnish co-authors at the Materials Physics Laboratory, namely prof. Martti Salomaa and M.Sc. Juha Vartiainen, for fruitful collaboration. In particular, I am indebted to prof. Salomaa for making my work on quantum computing possible. Enlightening discussions with M.Sc. Teemu Ojanen and M.Sc. Mikko Möttönen in the "Theory Room" are gratefully acknowledged.

Since the beginning of the year 2003 I have worked in the Quantronics group lead by Dr. Panu Helistö at Microsensing of VTT Information Technology. Almost from the beginning of 2003 I have also had the opportunity to broaden my perspective on physics by working partially in acad. prof. Jukka Pekola's group in the Low Temperature Laboratory at HUT. This arrangement has proven more than great. I am extremely grateful to acad. prof. Pekola for his dedicated guidance. I would also like to thank my group members at VTT and in particular prof. Heikki Seppä for guidance and stimulating discussions. In addition, I would like to thank M.Sc. Jani Kivioja for the long but fun days that we have spent next to the cryostat. I am also grateful to those who I have not explicitly mentioned but who have been helpful along the way.

I wish to thank the Research Foundation of Helsinki University of Technology for funding my Master's Thesis work. I would also like to thank the Academy of Finland for funding during my time in the Materials Physics Laboratory through the Graduate School in Technical Physics. Since 2003, my research has been funded by VTT internal funding and the Academy of Finland for which I am grateful. I would also like to acknowledge the European Science Foundation PiShift program, the EU-IST-FET SQUBIT, and the Magnus Ehrnrooth Foundation for travel support. The excellent computing resources of CSC Finland are gratefully acknowledged.

I would also like to thank my parents Juha and Merja for support and everything else during my 26+ years. Thanks go also to my brother Ville and sister Johanna. Finally, the greatest of thanks go to my wife Katriina and our little wonder girl Alina.

List of Publications

This Thesis is a review of the author's work on the control of the temporal evolution of quantum systems in general and of Josephson junction systems in particular. It consists of an overview and the following publications:

I. A. O. Niskanen, M. Nakahara, and M. M. Salomaa, *Realization of arbitrary gates in holonomic quantum computation*, Physical Review A **67**, 012319 (2003).

II. A. O. Niskanen, M. Nakahara, and M. M. Salomaa, *Optimal holonomic quantum gates*, Quantum Information and Computation **2**, 560–577 (2002).

III. A. O. Niskanen, J. J. Vartiainen, and M. M. Salomaa, *Optimal multiqubit operations for Josephson charge qubits*, Physical Review Letters **90**, 197901 (2003).

IV. J. J. Vartiainen, A. O. Niskanen, M. Nakahara, and M. M. Salomaa, *Acceleration of quantum algorithms using three-qubit gates*, International Journal of Quantum Information **2**, 1–10 (2004).

V. J. J. Vartiainen, A. O. Niskanen, M. Nakahara, and M. M. Salomaa, *Implementing Shor's algorithm on Josephson charge qubits*, Physical Review A **70**, 012319 (2004).

VI. A. O. Niskanen, J. P. Pekola, and H. Seppä, *Fast and accurate single-island charge pump: Implementation of a Cooper pair pump*, Physical Review Letters **91**, 177003 (2003).

VII. A. O. Niskanen, J. M. Kivioja, H. Seppä, and J. P. Pekola, *Evidence of Cooper pair pumping with combined flux and voltage control*, submitted, 4 pages (2004); cond-mat/0410758.

Throughout the overview the above articles are referred to by their Roman numerals.

Author's Contribution

The research reported in this Thesis has been carried out in the Materials Physics Laboratory at Helsinki University of Technology in 2002 (Publications I–III) and in 2003–2004 (Publications VI and VII) jointly at Microsensing of VTT Information Technology and the Low Temperature Laboratory at Helsinki University of Technology. During 2003–2004 the author has also continued, out of academic interest, part-time the research initiated at the Materials Physics Laboratory in 2002 (Publications IV and V).

The author has had a central role in all aspects of the work reported in this Thesis. The author has written the manuscripts for Publications I–III, VI and VII and actively participated in writing Publications IV and V. The computer programs used in Publications I, II and VI were developed by the author. The author was a co-developer of the parallel programs and methods used in Publications III–V, which are based on the author's original sequential algorithms used in Publications I and II. Publication VI, the theory of the Cooper pair "sluice", is based on the author's original idea. Publication VII is a report of the experimental verification of this idea. The author fabricated the samples used in the experiment, actively participated in the low-temperature measurements and analyzed the data of Publication VII.

In addition, the author has presented the results of the work at major international conferences including the Erato Workshop on Quantum Information Science (EQIS) in Tokyo (Japan) 2002, the 6^{th} European Conference on Applied Superconductivity (EUCAS) in Sorrento (Italy) 2003 and the 39^{th} Rencontres de Moriond on Quantum Information and Decoherence in Nanosystems in La Thuile (Italy) 2004. Some results of the Thesis were also presented in the Applied Superconductivity Conference (ASC) in Jacksonville (Florida, USA) 2004.

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Appendices: Publications I–VII

1 Introduction

The temporal control of pure quantum systems has two competing requirements. On one hand, it is desired that the system under scrutiny is well isolated from its environment such that the dynamics may be assumed to be unitary. On the other hand, however, any temporal control implies a time dependence in the Hamiltonian which can only be an effective approximation and a result of an interaction with the environment such that the system cannot stay pure indefinitely. Despite this, ever since the emergence of Shor's algorithm [1] for factoring large composite integers on a quantum computer [2–5] the control of the temporal evolution of quantum systems has been a topic of intensive investigations in physics. The "killer application" of Shor's algorithm would be the breaking of the RSA cryptosystem. This could have a remarkable societal impact, and not necessarily a negative one. To complement the possible emergence of a quantum computer, quantum cryptography [6] is quite advanced already today. Nevertheless, in order to perform calculations on a quantum computer, the quantum programmer needs to have full control over the time-evolution of the system. Moreover, the system needs to stay pure in the quantum-mechanical sense. It is possible to have quantum control that does not maintain the purity, and the difference between the control of an impure state and that of a pure state should be distinguished. Roughly speaking, in the control of pure states not only the probabilities of different states but also the quantum-mechanical phases are of interest. This Thesis discusses the control of pure or almost pure quantum systems.

Quantum control has been studied in the past particularly in the context of nuclear magnetic resonance (NMR) [7] and, e.g., within molecular dynamics [8]. Quite complicated quantum-computing experiments have also been carried out in NMR with the most spectacular achievement of a seven-qubit algorithm for factoring the number fifteen [9]. The topic of controlling the macroscopic quantum state of a system such as the nanoelectronic superconducting Cooper pair box [10] is less thoroughly explored. Nevertheless, many steps have been taken in recent years towards an experimental realization of a Josephson junction based quantum computer. In the experiments by Nakamura et al. [11–13], the coherent oscillations of a Cooper pair box were first observed. The coherent operation of a coupled Cooper pair box system has also been demonstrated [14, 15]. The dual realization, i.e. the superconducting qubit taking advantage of the flux degree of freedom [16, 17] has been experimentally verified as well [18, 19]. The macroscopic coherent behavior of a current-biased large Josephson junction, or the phase qubit, was recently realized [20, 21] with as high as μs coherence times reported in Ref. [20]. Coherence times on the same order were measured in the so-called quantronium circuit [22] in Saclay. A generalization of the current-biased Josephson junction, the current-biased SQUID, has also been demonstrated to exhibit coherent behavior [23]. Exotic scenarios, such as the tetrahedral qubit [24], have been suggested as well. For a review of various superconducting qubits up to year 2001 see in particular Ref. [25].

The control of adiabatic Cooper pair pumps (CPPs) [26–28] is an instance of the geometrical control of a superconducting system similar to superconducting qubits. While in

superconducting qubits the control is typically achieved via ordinary dynamical temporal evolution, the CPPs are controlled adiabatically and cyclically such that no transitions between states occur. In quantum computing unitary transformations are pursued while in Cooper pair pumping the time-integral of the current is of interest. It is however possible, at least in principle, to achieve also general unitary transformations via adiabatic evolutions as holonomies. This branch of quantum information is called holonomic quantum computing (HQC) [29]. This Thesis contains examples of both adiabatic and dynamical quantum computing as well as Cooper pair pumping.

The Overview is organized as follows. Section 2 briefly discusses the unitary evolution of quantum systems in general and the concept of geometrical evolution in particular. Section 3 discusses the optimization of quantum algorithms developed in detail in Publications I–V. Finding unitary operations within a realization-independent model of holonomic quantum computing (Publications I and II) is studied first. Then the construction of dynamical quantum gates (Publications III–V) for a model identical to a Cooper pair box array is explored. The highlight of the Section is a theoretical study of carrying out the simplest nontrivial application of Shor's factorization algorithm on Josephson charge qubits. The topic of Section 4 is the adiabatic Cooper pair pump and especially the so-called Cooper pair "sluice" of Publications VI and VII. This topic is an illustration of the multitude of present-day applications achievable with almost identical techniques and structures as those intended to be used in quantum computing. As explained below this device aimed at a metrological application has many common features with superconducting qubits and it is further closely related to the concept of Berry's phase. Cooper pair pumping has been studied extensively in the past but has never proven even nearly as accurate as, e.g., single-electron pumping [30]. The sluice is hoped to bridge this gap. Finally, Section 5 is dedicated to a discussion of the results in this Thesis.

2 Controlled Evolution of Quantum Systems

The topics discussed in this Thesis rely on the cyclic control of quantum systems achieved via manipulating their Hamiltonians in time. That is, in all the applications considered the parameters of a Hamiltonian go around loops in the parameter space in order to achieve some desired effect. These controlled cyclic temporal evolutions may roughly be divided into two main categories: Evolution may be either dynamical or geometrical in nature. Geometrical evolution may arise if the time dependence is slow enough compared to the relevant energy level separations, i.e., all the controllable parameters of the Hamiltonian are tuned adiabatically. As the term geometrical implies, only the geometry of the loop matters and not the speed at which it is traversed. Geometrical, or adiabatic, evolutions may further be divided into Abelian and non-Abelian ones. Abelian evolutions are commuting, i.e. the order in which the loops are arranged does not matter, while non-Abelian evolutions do not commute. Abelian evolutions give rise to Berry's phase [31] while non-Abelian evolutions may not be characterized by a simple phase but rather unitary matrices are needed as pointed out by Wilczek and Zee [32]. They are called holonomies.

Decoherence mechanisms and open quantum systems (see, e.g., Ref. [33, 34]) are not considered in detail in this Thesis. Many studies on the decoherence mechanisms in superconducting circuits exist in the literature, see e.g. Refs. [25, 35–39] and references therein. In Subsection 2.1 below we give a brief introduction to the concepts of quantum mechanics that are important for the present work including general dynamical evolution. We then proceed to discuss geometrical evolution in Subsection 2.2. For a critical discussion of the fundamentals of quantum mechanics, see e.g. Ref. [40]. Publications I, II, VI and VII are related to adiabatic evolution while Publications III–V discuss dynamical evolutions.

2.1 Quantum mechanics and dynamical temporal evolution

The state of a pure quantum system is described by a state vector $|\psi\rangle$ in a complete inner-product space called the Hilbert space. A physical state vector $|\psi\rangle$ can always be normalized to unity $\langle\psi|\psi\rangle = 1$. It may occur, however, that the state is not pure but rather mixed in which case the system is described with a state operator, or a density matrix (operator) ρ with $\mathrm{Tr}\,\rho = 1$. The system is pure if and only if $\mathrm{Tr}\,\rho^2 = 1$ in which case one may use the state vector to describe the system. Given a state vector, the corresponding density operator may be formed via $\rho = |\psi\rangle\langle\psi|$. The state vector and the state operator are not themselves directly observable quantities in quantum mechanics. Namely, every observable has an associated self-adjoint operator $\mathcal{O} = \mathcal{O}^\dagger$. In the spirit of the statistical interpretation of quantum mechanics, the expectation value for the k^{th} moment of an observable is given by either $\langle\mathcal{O}^k\rangle = \mathrm{Tr}\,\left(\rho\mathcal{O}^k\right)$ or alternatively by $\langle\mathcal{O}^k\rangle = \langle\psi|\mathcal{O}^k|\psi\rangle$ in the special case of a pure system. The measurement of the observable always yields an eigenvalue of the operator $\mathcal{O}$. Even if the state $|\psi\rangle$ is not an eigenstate of $\mathcal{O}$, then owing to the self-adjointness of $\mathcal{O}$ we may utilize the complete

eigenbasis to expand the state. That is, we may write

$$|\psi\rangle = \sum_{\alpha} c_\alpha |\psi_\alpha\rangle, \tag{1}$$

where $\mathcal{O}|\psi_\alpha\rangle = \omega_\alpha|\psi_\alpha\rangle$, $\sum_\alpha |c_\alpha|^2 = 1$, $\langle\psi_\beta|\psi_\alpha\rangle = \delta_{\alpha\beta}$ and $\omega_\alpha \in \mathbb{R}$. An ideal projective measurement will result in ω_α with the probability $|c_\alpha|^2$. Immediately following the measurement, the system will reside in the state $|\psi_\alpha\rangle$.

For every quantum system, there exists a Hamiltonian operator $\mathcal{H}$ which describes the energy of the system. This dictates the exact form of the temporal evolution. Namely, the dynamics of an isolated quantum system is governed by the Schrödinger equation

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = \mathcal{H}|\psi(t)\rangle. \tag{2}$$

The corresponding equation for the density operator is

$$i\hbar\dot{\rho}(t) = [\mathcal{H}, \rho]. \tag{3}$$

For a time-independent Hamiltonian Eq. (2) may be simply solved using operator exponentiation, i.e. $|\psi(t_1)\rangle = \exp(-i\mathcal{H}(t_1 - t_0)/\hbar)|\psi(t_0)\rangle$. If the Hamiltonian has a general time dependence $\mathcal{H} \equiv \mathcal{H}_{\mathbf{q}(t)}$ the situation is considerably more complicated since the Hamiltonian may have a non-vanishing commutator with itself at different instants of time. In this work the Hamiltonian is taken to depend on a set of tunable parameters. These parameters are described by a vector-valued function of time $\mathbf{q}(t)$. This vector naturally contains all the parameters that we have control over. We can, even then, still formally solve for the time evolution using the time-ordering operator $\mathcal{T}$, which results in

$$|\psi(t_1)\rangle = \mathcal{T}\exp\left(-i\int_{t_0}^{t_1}\mathcal{H}_{\mathbf{q}(t)}dt/\hbar\right)|\psi(t_0)\rangle. \tag{4}$$

In spite of the integral, the above expression does not involve integration in the ordinary sense but it is rather a product integral. The effect of $\mathcal{T}$ is to arrange a sequence of operators, each of which is associated with an instant in time, such that the operators associated with earlier times are always to the right from those associated with later instants. Regardless of the exact details, however, the dynamics of an isolated quantum system is always unitary. We may write $|\psi(t_1)\rangle = U(t_1, t_0)|\psi(t_0)\rangle$ where in the general case the unitary operator $U(t_1, t_0)$ is given by

$$U(t_1, t_0) = \mathcal{T}\exp\left(-i\int_{t_0}^{t_1}\mathcal{H}_{\mathbf{q}(t)}dt/\hbar\right). \tag{5}$$

Due to unitarity, the quantum-temporal evolution of a closed system is always reversible: $U(t_1, t_0)^{-1} = U(t_1, t_0)^\dagger$. The norm is also preserved, i.e.

$$\langle\psi(t_1)|\psi(t_1)\rangle = \langle\psi(t_0)|U(t_1, t_0)^\dagger U(t_1, t_0)|\psi(t_0)\rangle = \langle\psi(t_0)|\psi(t_0)\rangle = 1, \tag{6}$$

which is consistent with the probability interpretation of quantum mechanics. The unitary temporal evolution of a mixed state may be expressed also very concisely as $\rho(t_1) = U(t_1, t_0)\rho(t_0)U(t_1, t_0)^\dagger$.

Equation (5) is quite general and comprises all forms of unitary evolution, i.e. both adiabatic and non-adiabatic behaviors. It serves as the natural starting point for numerical calculations. Depending on the application, one either aims at realizing a certain unitary evolution (quantum computing) or a certain consequence of evolutions (e.g., quantum pumping). The unitarity of the temporal evolution only breaks down when the system in consideration is no longer isolated. The quantum measurement mentioned briefly above is clearly non-unitary and, as a matter of fact, it is just through interactions that the actual measurements take place. This brings us to the problem of combining quantum systems. Two quantum systems with separate Hilbert spaces may be combined by considering their tensor product. That is, for any $|\psi_1\rangle$ (ρ_1) and $|\psi_2\rangle$ (ρ_2) the combined state is $|\psi_1\rangle \otimes |\psi_2\rangle$ ($\rho_1 \otimes \rho_2$). In the case of finite-dimensional spaces the tensor product is just the Kronecker product for matrices. The total Hamiltonian is, on the other hand $\mathcal{H}_{\text{tot}} = \mathcal{H}_1 \otimes I + I \otimes \mathcal{H}_2$. However, it may be that the two systems are non-isolated such that the total Hamiltonian may not be written as a sum of two terms each of which acts non-trivially only on the subspace of one of the systems but rather $\mathcal{H}_{\text{tot}} = \mathcal{H}_1 \otimes I + I \otimes \mathcal{H}_2 + \mathcal{H}_{\text{int}}$. It may also be the case that two initially separate pure systems cannot be described by $|\psi_1\rangle \otimes |\psi_2\rangle$. Then the total system is called entangled. To obtain the state operator for a certain subsystem of a possibly entangled total system one simply traces over the degrees of freedom of the uninteresting part of the Hilbert space. That is, if we have two systems 1 and 2, then $\rho_1 = \text{Tr}_2\rho$ is the state operator of subsystem 1. This partial trace combined with unitary global evolution may result in non-unitary temporal evolution.

2.2 Geometrical temporal evolution

In the special case when the temporal evolution of a quantum system may be considered to be adiabatic, Eq. (5) may be further refined. Adiabaticity in quantum mechanics means that if the quantum system in question, described by some Hamiltonian $\mathcal{H}_{\mathbf{q}(t)}$, is initially in the k^{th} eigenstate of energy, then we may also assume that it stays in the corresponding k^{th} eigenstate. This is the case when the dynamics is slow compared to the energy-level separations. Clearly no level crossings can be allowed such that the ordering of the states is possible and the separations remain nonzero. In this Thesis we consider only adiabatic systems in the ground state. Thus, for our purposes, the adiabaticity criterion means that all the related frequencies are much lower than the resonant frequency between the ground state and the first exited state. This resonant frequency may of course also depend on time, and thus the condition must hold at all times.

This basic assumption has quite nontrivial consequences [31,32,41]. For our purposes it is sufficient to concentrate on what happens to the ground state. Let us assume that the ground state has g degenerate eigenstates denoted by $|0\alpha;\mathbf{q}\rangle$ ($\alpha = 1, ..., g$) and that no level crossings occur at least between the ground state and the higher excited states. The eigenvalue of the ground state is $\varepsilon_{\mathbf{q}}$, such that

$$\mathcal{H}_{\mathbf{q}}|0\alpha;\mathbf{q}\rangle = \varepsilon_{\mathbf{q}}|0\alpha;\mathbf{q}\rangle \tag{7}$$

and

$$\langle 0\alpha;\mathbf{q}|0\beta;\mathbf{q}\rangle = \delta_{\alpha\beta}. \tag{8}$$

Moreover, the eigenvectors of the ground-state subspace are also orthogonal to the higher excited states. Let us assume that the state of the system is initially any one of orthonormal ground states $|\alpha;\mathbf{q}(t_0)\rangle$ and that the system evolves adiabatically over time $t \in [t_0, t_1]$ and also that the parameters go around a loop such that $\mathbf{q}(t_0) = \mathbf{q}(t_1)$. Then we may write the state of the system $|\psi_\alpha(t)\rangle$ at time t as

$$|\psi_\alpha(t)\rangle = \sum_{\theta=1}^{g} U_{\theta\alpha}(t,t_0)|0\theta;\mathbf{q}(t)\rangle \tag{9}$$

with some complex coefficients $U_{\beta\alpha}(t,t_0)$ that must satisfy $U_{\beta\alpha}(t_0,t_0) = \delta_{\beta\alpha}$. Plugging this into the Schrödinger equation, multiplying from the left by $\langle 0\beta;\mathbf{q}(t)|$ and using the orthonormality of the states yields

$$\frac{dU_{\beta\alpha}(t,t_0)}{dt} = -\sum_{\theta=1}^{g}\langle 0\beta;\mathbf{q}(t)|\frac{d}{dt}|0\theta;\mathbf{q}(t)\rangle U_{\theta\alpha}(t,t_0) - i\varepsilon_{\mathbf{q}(t)}U_{\beta\alpha}(t,t_0)/\hbar. \tag{10}$$

This has the solution

$$U(t,t_0) = e^{-i\int_{t_0}^{t}\varepsilon_{\mathbf{q}(\tau)}d\tau/\hbar}\mathcal{T}\exp\left(-\int_{t_0}^{t}\mathbf{A}(\tau)d\tau\right), \tag{11}$$

where $\mathbf{A}(t)$ is a matrix whose entries $\mathbf{A}_{\beta\alpha}(t)$ are given by

$$\mathbf{A}_{\beta\alpha}(t) = \langle 0\beta;\mathbf{q}(t)|\frac{d}{dt}|0\alpha;\mathbf{q}(t)\rangle. \tag{12}$$

Neglecting the dynamical phase $\theta_{\text{dyn}} = -\int_{t_0}^{t}\varepsilon_{\mathbf{q}(\tau)}d\tau/\hbar$ for now and introducing the connection matrices $\mathcal{A}_i$ whose elements are

$$\mathcal{A}_{i;\beta\alpha} = \langle 0\beta;\mathbf{q}|\frac{\partial}{\partial\mathbf{q}_i}|0\alpha;\mathbf{q}\rangle \tag{13}$$

allows us to rewrite Eq. (11) at the instant $t = t_1$ as

$$U(t_1,t_0) \equiv U_\gamma = \mathcal{P}\exp\left(-\oint_\gamma \mathcal{A}_i d\mathbf{q}^i\right), \tag{14}$$

where γ is the loop around which we traverse. The quantity $\mathcal{A}_i d\mathbf{q}^i$ is sometimes called the Wilczek-Zee connection one-form. Einstein's summation convention over all the components of the control parameter vector, i.e. the index i, is assumed. The path-ordering operator $\mathcal{P}$ is used above. Its operation is similar to that of $\mathcal{T}$.

Now if instead of the state $|\alpha;\mathbf{q}(t_0)\rangle$ we were initially to start from an arbitrary superposition $\sum_{\alpha=1}^{g} c_\alpha|\alpha;\mathbf{q}(t_0)\rangle$ then at time t_1 the state of the system would be

$$|\psi(t_1)\rangle = \sum_{\alpha=1}^{g} c_\alpha|\psi_\alpha(t_1)\rangle \tag{15}$$

or

$$|\psi(t_1)\rangle = \sum_{\alpha,\beta=1}^{g} U_{\beta\alpha}(t_1,t_0)c_\alpha|\beta;\mathbf{q}(t_1)\rangle = \sum_{\alpha,\beta=1}^{g}(U_\gamma)_{\beta\alpha}c_\alpha|\beta;\mathbf{q}_0\rangle. \tag{16}$$

We see form this that U_γ is indeed the unitary matrix that describes how the quantum state evolves during each loop based at $\mathbf{q}(t_0)=\mathbf{q}_0$. This is called a non-Abelian holonomy [32,41] in the degenerate case (Publications I and II) and Berry's phase [31] (Publications VI and VII) in the nondegenerate case, i.e. $U_\gamma = e^{i\theta_{\text{Berry}}}$ if $g=1$. In the nondegenerate case we may denote the ground state simply as $|0;\mathbf{q}\rangle$ and since the path ordering is then meaningless, Berry's phase is simply

$$\theta_{\text{Berry}} = i\oint_\gamma \langle 0;\mathbf{q}|\frac{\partial}{\partial\mathbf{q}_i}|0;\mathbf{q}\rangle d\mathbf{q}^i = i\oint_\gamma \langle 0;\mathbf{q}(t)|\nabla_{\mathbf{q}}|0;\mathbf{q}(t)\rangle\cdot d\mathbf{q}. \tag{17}$$

Thus, the cyclic quantum evolution of the ground state in the adiabatic limit has two contributions; the more-or-less trivial dynamical factor $e^{-i\int_{t_0}^{t_1}\varepsilon_{\mathbf{q}(t)}dt/\hbar}$ that can be neglected in e.g. quantum computing applications and the geometrical contribution U_γ. To obtain some desired holonomic evolution one needs to describe a loop γ in the parameter space spanned by all the controllable parameters. Whereas in general the speed at which a loop is traversed plays a role, in the adiabatic evolution only the geometry of the path (not its parameterization) matters. It may appear at first sight that for a nondegenerate system in its ground state, Berry's phase would be meaningless since it only describes a global phase. This is not the case as will be seen in Section 4 where we discuss Cooper pair pumps. For universal quantum computation based solely on ground-state adiabatic control, however, a degenerate system is required.

3 Optimization of Quantum Algorithms

Quantum computing is potentially a very spectacular application of the temporal control of quantum systems. Basically any collection of two-state (or more) quantum systems that can be controlled, and moreover, the couplings of which we have control over, or can take into account somehow, is a potential quantum computer. Provided that the quantum system is sufficiently well isolated from its environment, we may assume the dynamics to be unitary as in the previous Section. However, the parameters of the Hamiltonian need to be tunable and thus the isolation must not be perfect. In this Section we shall first introduce the concept of quantum computing. Many excellent overviews of this subject may be found in the literature, see e.g. Refs. [2–5]. It will turn out that a quantum algorithm is nothing but a unitary operator. It is programmed by finding a proper control pulse $\mathbf{q}(t)$ and executed by applying the pulse on the quantum system. In Subsection 3.2 we consider a realization–independent approach for finding physical implementations of holonomic quantum computations. Subsection 3.3 describes a similar approach for finding optimized logical dynamical quantum gates on Josephson charge qubits. All the methods presented rely on intensive numerical optimization. The key point of this Section is that instead of using sequences of elementary operations, we pursue a method of finding direct implementations of single and multiple qubit operations in a single pulse sequence. We demonstrate that it is in practice much more advantageous to implement a quantum algorithm via first finding, using ordinary computers, a direct implementation for as large a multiqubit operation as possible and then implementing this optimized operation on a quantum computer rather than using some limited set of elementary operations.

3.1 Quantum computing

Quantum computers can solve certain problems that are classically considered to require exponential resources (time and space) in polynomial time and space. The idea of quantum computing is to take advantage of the global properties of a very high-dimensional multi-partite Hilbert space. A quantum computer is a quantum system typically consisting of multiple two-state subsystems called quantum bits, or qubits. A prototype for a qubit is the spin degree of freedom of a spin-1/2 particle. Information is encoded in the states of the qubits such that one state of the qubit corresponds to the "0" of a classical digital bit while the other corresponds to "1". Let us denote the basis states of the collection of N qubits by $|0_j\rangle$ and $|1_j\rangle$ with $j \in \{1, \ldots, N\}$. One often uses the vector notation

$$|0_j\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |1_j\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{18}$$

for these states. If the states of the individual qubits are $|\psi_j\rangle$ with $\psi_j = 0, 1$ then the state of the composite system may be expressed using the tensor product as

$$|\Psi\rangle = \bigotimes_{j=1}^{N} |\psi_i\rangle = |\psi_N\rangle \otimes \ldots \otimes |\psi_1\rangle = |\psi_N \ldots \psi_1\rangle \,, \tag{19}$$

where the last form is an often used abbreviation. In the absence of superpositions the quantum information contained in this quantum register is interpreted just like the information in a classical bit register; the data is just a binary number. The strength of a quantum computer, however, emerges from the fact that the quantum register may evolve into a superposition of all the possible 2^N states. That is, if $|\Psi_\alpha\rangle$ is some N-qubit state corresponding to a binary number, then the state of the quantum computer can be

$$|\Psi\rangle = \sum_{\alpha=1}^{2^N} c_\alpha |\Psi_\alpha\rangle \,, \tag{20}$$

with $\langle\Psi|\Psi\rangle = 1$. The prototype of an entangled superposition is the so-called Bell state for two qubits

$$|\Psi\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle \right). \tag{21}$$

The interpretation of the data contained in this register is entirely non-classical; with probability one half the bits are either both zeros or ones. Moreover, the measurement of one of the qubits immediately tells us the result that the measurement of the second qubit would give. This has some very counterintuitive implications and the interpretation of this kind of state even confused Einstein [42]. Entangled states, such as the Bell state above, can be used for so-called (deterministic) quantum teleportation that has been recently realized using ion traps [43, 44].

The quantum algorithm is nothing but a 2^N-dimensional unitary operator of Eq. (5) which dictates the temporal evolution of the quantum register, i.e.

$$|\Psi(t_1)\rangle = U(t_1, t_0)|\Psi(t_0)\rangle. \tag{22}$$

The evolution of the quantum computer is governed by the Hamiltonian $\mathcal{H}_{\mathbf{q}(t)}$ whose time-dependence the experimenter must have control over. The control is mediated by the parameters $\mathbf{q}(t)$ and different formal expressions for the algorithm U can be derived as discussed in the previous Section. Clearly the number of degrees of freedom for the algorithm is immense; it takes $2^{2N} - 1$ real numbers to describe the most general kind of an algorithm while for applications $N \gg 100$. Luckily, practical algorithms exist too. Typically, we would desire the operator U to perform, for instance, the quantum part of Shor's algorithm [1] or the Grover search [45] both of which can be carried out by applying a polynomial number of so-called elementary operations [46]. Shor's algorithm can factor large integers in polynomial time, which is otherwise believed to be exponentially hard, while Grover's search can be used to carry out a database search of an unsorted database in time proportional to the square root of the entries in it. The best known decompositions of arbitrary multiqubit gates have been reported in Refs. [47, 48] but, nevertheless, the number of required gates scales exponentially with the number of qubits.

The unique property of quantum mechanics that makes quantum computing attractive is that unitary operator "processes" all orthogonal basis states independently. In other words, the quantum algorithm may process 2^N different inputs at once if the register is initialized for instance in an equal superposition. This is sometimes called quantum

parallelism. The task carried out e.g. in Shor's algorithm is the evaluation of a certain modular function, see e.g. Refs. [1, 2] or Paper V. With $N \sim 10^3$ the number of states is already immense and beyond the capacity of all classical computers. However, after the unitary temporal evolution one has to measure the state of the system. Each qubit is found in either the state $|0\rangle$ or $|1\rangle$. If the state of the register prior to measurement is $|\Psi\rangle$, then the probability of obtaining the result $|\tilde{\Psi}\rangle = \bigotimes_{j=1}^{N} |\tilde{\psi}_j\rangle$ ($\tilde{\psi}_j = 0$ or $\tilde{\psi}_j = 1$) is given by

$$P(\Psi) = \langle\Psi|\tilde{\Psi}\rangle\langle\tilde{\Psi}|\Psi\rangle = |\langle\Psi|\tilde{\Psi}\rangle|^2. \tag{23}$$

This is the tricky part. No matter how many orthogonal basis states have non-vanishing amplitudes in the superposition, upon measurement only one of them survives. Moreover, the result is stochastic. The quantum measurement makes it impossible to obtain more than one output. The trick that can be used then is to further process the information in the quantum register before measurement and to look for "global" properties in it. In Shor's algorithm one is interested in the period of the modular function and luckily the quantum equivalent of the fast Fourier transform may be carried out efficiently. This causes the quantum register to form strong interference patterns and upon measurement it is possible, stochastically, to deduce the period. Thus the true strength of quantum computing is only unleashed in a certain class of applications in which some well-defined global property is known.

We list the requirements for practical quantum computing following DiVincenzo [49]. One needs to have:

- a scalable physical system with well characterized qubits
- the ability to initialize the state of the qubits to a simple fiducial state
- long relevant decoherence times, much longer than the gate operation time
- a universal set of quantum gates
- a qubit-specific measurement capability.

All of these points are necessary and it seems that all the existing suggestions for physical realizations of quantum computing possess strengths in some of these areas but not in each one of them. In this work we are primarily interested in how to carry out the unitary transformations, i.e. the quantum gates.

As mentioned above, typically the unitary operator U is decomposed into a sequence of so-called elementary gates [46] that act non-trivially only on one or two qubits. These are analogous with the basic logical operations of an ordinary computer. The physical implementation for these is often found by hand and the Hamiltonian is sometimes even considered piecewise constant in time. This leads to abrupt switchings in the parameter sequences which are hard if not impossible to implement. Finite rise and fall times of real pulses lead to errors [50]. Furthermore, in general only a limited number of logically different gates are assumed to be available. Thus the logical gate sequences may get prohibitively long. In the next two subsections methods for finding arbitrary single and

multiple qubit gates avoiding abrupt switchings are considered. The motivation for this is that the more complicated gates we may perform in a single step, the more of the valuable execution time we save. This is extremely important due to the presence of decoherence which inevitably limits the total execution time of the algorithm. In Subsection 3.2, methods for finding the adiabatic loop γ in the control-parameter space for any one-qubit and two-qubit operation for a certain toy model is presented, while in Subsection 3.3 control sequences realizing up to three-qubit operations for Josephson charge qubits are found. The developments presented here have recently obtained experimental verification when Nakahara et al. demonstrated [51] the acceleration of the two-qubit Grover search at best by four times by first optimizing the algorithm and then by carrying it out experimentally in an NMR setup.

3.2 Adiabatic non-Abelian quantum gates

Holonomic quantum computing (HQC) [29, 52–55] is a subfield of quantum information processing in which the quantum register is assumed to be fully degenerate and the quantum control is implemented using Eq. (14). The reason for studying holonomic quantum computing is that it is hoped to be robust against decoherence due to the degeneracy of the spectrum. A clear benefit is also the fact that the exact timing of the pulses is not crucial since the evolution is purely geometrical as long as the adiabaticity is maintained. Additional features include the absence of unwanted phases on idle qubits that inevitably accumulate in any scenario in which the logical states are energetically different.

Thus in HQC each unitary gate is associated with a loop in the parameter space, and a sequence of loops forms the full quantum algorithm. Holonomic or adiabatic non-Abelian gates in a three-state model are studied in papers I and II. The results obtained are quite general and are not limited to any particular physical system. For various suggestions for the realization of non-Abelian holonomies with Josephson junction structures, see Refs. [56–58]. Also optical [59] and semiconductor [60] HQC has been suggested. Berry's Abelian geometrical phase has been envisaged to be used for universal quantum computation in superconducting systems by Falci et al. [61], but there the system under study is not in the ground state such that differences in Berry phases are of interest and, furthermore, sudden changes in the parameters are also used. In HQC purely ground state systems and strictly adiabatic control is used.

The problem considered is the following: Given a unitary quantum gate $\hat{U}$, what is the parameter loop γ that produces $\hat{U}$ through Eq. (14), i.e. under which conditions $U_\gamma = \mathcal{P}\exp\left(-\oint_\gamma \mathcal{A}_i d\mathbf{q}^i\right)$ equals $\hat{U}$? It is straightforward to solve the direct problem but the solution of the inverse problem turns out to involve heavy computations. However, this is clearly the relevant question from the point of view of holonomic quantum computing since γ is just the experimental control sequence. A possible way of finding a path γ that realizes $\hat{U}$ is to use numerical optimization. Namely, let us define

$$f(\gamma) = \|\hat{U} - U_\gamma\|, \tag{24}$$

where $\|\cdot\|$ is some specified norm. In this Thesis we use the Frobenius norm $\|\cdot\|_F$ defined as $\|\mathbf{A}\|_F = \sqrt{\mathrm{Tr}\,(A^\dagger A)}$. Then finding the minimum of $f(\gamma)$, which clearly is equal to zero if a solution to the original problem exists, is equivalent to finding a path γ that implements $\hat{U}$. In practice, the multidimensional path is conveniently discretized for instance into polygonal loops, i.e., into loops that have a finite number of vertices between which one interpolates linearly. Then we are effectively searching for the minimum in a subspace of all (continuous) loops and the coordinates of the vertices serve as natural optimization variables. Various numerical algorithms for the minimization are possible, but the so-called polytope search [62] was found to be particularly successful for the problem. Exact methods have been studied also for the solution of a similar problem [63].

The functional evaluations for a given polygonal path may easily be carried out by the discretization of the path and considering the connection coefficients $\mathcal{A}_i$ piecewise constant such that evaluation of U_γ reduce to multiplication of matrix exponentials. That is, for a discretization $\gamma_1, \ldots, \gamma_n$ of the loop γ we may write

$$U_\gamma \approx \exp(-\sum_i \mathcal{A}_i(\gamma_n)\delta\gamma_n^i) \cdots \exp(-\sum_i \mathcal{A}_i(\gamma_1)\delta\gamma_1^i), \tag{25}$$

where $\mathcal{A}_i(\gamma_k)$ stands for the i^{th} connection component evaluated at the discretization point γ_k and $\delta\gamma_k^j$ is the finite difference of the j^{th} parameter component of the k^{th} interval. The number of connection components and thus the bounds on the summation index i depend on the number of controllable parameters. From this discretization it is clear why expressions of the kind appearing in Eqs. (14) and (5) are sometimes called product integrals; letting $n \to \infty$ and $\delta\gamma_k^j \to 0$ renders the approximation in Eq. (25) exact. The matrix exponentials may be either calculated using the Taylor expansion or the Cayley form, see Paper V. More details of the numerics can be found in publications I and II. In general, a realization for an arbitrary N-qubit gate is expected to exist if the number of degrees of freedom in the optimization exceeds the dimensionality of the Lie algebra $u(2^N)$ which is 2^{2N}.

Single-qubit gates

To get some concreteness to the problem we consider as an example a case where the individual qubits are encoded in the twofold degenerate ground state of a three-dimensional Hilbert space. We assume that the Hamiltonian is diagonal at the reference point $\mathbf{q}_0$ where the holonomy loops are based and the ground state energy is set to zero. Then the Hamiltonian at this point may be written simply as

$$\mathcal{H}_{\mathbf{q}_0} = \begin{pmatrix} \epsilon & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{26}$$

with $\epsilon > 0$. We then consider the adiabatic isospectral temporal dependence of the Hamiltonian to be of the form $\mathcal{H}_{\mathbf{q}} = W_{\mathbf{q}}\mathcal{H}_{\mathbf{q}_0}W_{\mathbf{q}}^\dagger$, where $W_{\mathbf{q}}$ is a unitary transformation that satisfies $W_{\mathbf{q}_0} = I_3$, where I_3 is the 3×3 identity matrix. All the temporal dependence of the Hamiltonian is encoded in $W_{\mathbf{q}}$ and this dependence is assumed to be adiabatic.

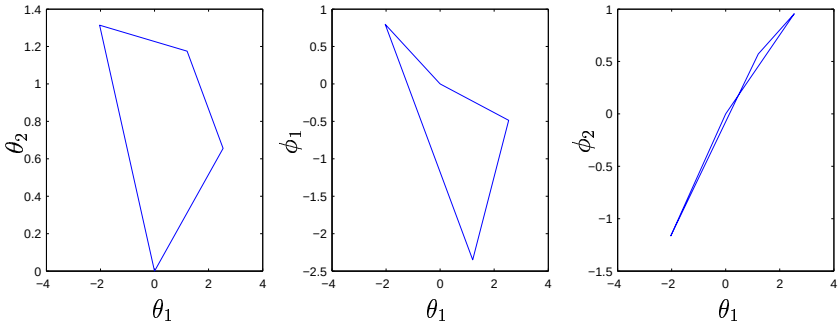

Figure 1. Loop in the parameter space that yields the gate $U = e^i \exp\left(i\frac{\pi}{7}\sigma_z\right) \exp\left(i\frac{1}{3}\sigma_y\right) \exp(i\sigma_z)$. *From Paper I.*

A convenient method to parameterize the unitary transformation $W_{\mathbf{q}}$ is to use the so-called Givens decomposition. It turns out that arbitrary rotations $W_{\mathbf{q}}$ are isomorphic to the complex projective space [64] $\mathbb{C}P^2$. This manifold may be parameterized using the four coordinates denoted θ_i and ϕ_i with $i = 1, 2$ in Papers I and II. The corresponding Wilczek-Zee matrices $\mathcal{A}_{\theta_i}$ and $\mathcal{A}_{\phi_i}$ can be found analytically and this allows one to write any holonomy on a single qubit as

$$U_\gamma = \mathcal{P} \exp\left(- \oint_\gamma \sum_{i=1}^{2} (\mathcal{A}_{\theta_i} d\theta_i + \mathcal{A}_{\phi_i} d\phi_i) \right). \tag{27}$$

The numerical calculations were carried using `Fortran 90` and the `IMSL` library. Figure 1 illustrates an example loop in the four-dimensional $(\theta_1, \theta_2, \phi_1, \phi_2)$-space for realizing a particular unitary operation, namely $U = e^i \exp\left(i\frac{\pi}{7}\sigma_z\right) \exp\left(i\frac{1}{3}\sigma_y\right) \exp(i\sigma_z)$. Here σ_z and σ_x are Pauli matrices and $\mathbf{q}_0 = (0, 0, 0, 0)^T$. Papers I and II report realizations for various other gates. The conclusion regarding single-qubit gates in the present setting is that they can all be found with a sufficient amount of flexibility in the paths.

Two-qubit gates

Two-qubit gates may also be found for HQC. To this end a way of coupling the qubits is desired. We define the two-qubit reference Hamiltonian to be

$$H_{\mathbf{q}_0}^{\text{2-qubit}} = \mathcal{H}_{\mathbf{q}_0} \otimes I_3 + I_3 \otimes \mathcal{H}_{\mathbf{q}_0}. \tag{28}$$

The most general kind of isospectral rotations for this 9-dimensional Hamiltonian is very complicated but we shall consider the product of a purely two-qubit rotation and that of a tensor product of single-qubit rotations, i.e.

$$W_{\mathbf{q}} = W_{\mathbf{q}}^{\text{2-qubit}} (W_{\mathbf{q}}^a \otimes W_{\mathbf{q}}^b), \tag{29}$$

where $W_{\mathbf{q}}^a$ ($W_{\mathbf{q}}^b$) is the single-qubit rotation of the Hamiltonian of the qubit a (b) identical to that used in purely single-qubit operations. We take $W^{\text{2-qubit}}$ to be of the form $W^{\text{2-qubit}} = e^{i\xi|11\rangle\langle 11|}$. Thus the rotations of the two-qubit Hamiltonian are parameterized using the nine parameters $(\theta_i^c, \phi_i^c, \xi)$ with $i = 1, 2$ and $c = a, b$. Arbitrary two-qubit quantum gates may be found within this model, and various examples may be found in papers I and II.

The problem of coupling multiple qubits is difficult in general, but in the case of HQC it is particularly hard due to the stringent requirement of degeneracy. The coupling presented here is merely an example, albeit a convenient one.

Length optimization

The motivation for studying holonomic quantum gates numerically is not just the need to find implementations of arbitrary gates. Namely, it is possible also to optimize with respect to a more general type of an error functional. Paper II discusses the optimization of HQC with respect to the length of the path numerically. Recently, however, also the exact solution of the so-called isoholonomic problem has been provided for an arbitrary k-dimensional unitary gate within a Hilbert space with a dimension larger than $2k$ [65].

3.3 Non-adiabatic Josephson charge-qubit gates

The developments presented above in the context of holonomic quantum computation may easily be generalized also to "ordinary" dynamical quantum computing. The optimization of multiqubit gates for the so-called Josephson charge-qubit model is the topic of publications III, IV and V. The only practical difference in the numerical optimization scheme of the present problem and HQC is the evaluation of the unitary operator. Whereas Eq. (14) was used above, here we utilize Eq. (5). The evaluation of the unitary operator was carried out using parallel programming [66]. The motivation is the same though: It is desired that a more complicated gate could be realized in a single shot without evoking elementary gates. Josephson charge qubits are discussed in detail for instance in Refs. [25,67] and Publication V. For an introduction to Cooper pair tunneling and superconducting circuits see e.g. Refs. [68–70].

Physical model

Consider the Josephson junction circuit shown in Fig. 2. In Fig. 2(a) an individual Cooper pair box is shown. It consists of a small metallic superconducting island (typically aluminum cooled to some 20–50 mK) having sub-micron dimensions coupled to a superconducting lead through a SQUID loop. The SQUID loop consists of Josephson junctions that are, e.g., formed by an oxide layer between superconducting metallic films. Cooper pairs may not be found inside the layer but they can have a finite possibility for tunneling through, provided that the oxide is sufficiently thin and the area of the junction sufficiently large. The state of a Josephson junction may be described by the superconducting phase difference ϕ over it which is just the time-integral of voltage times

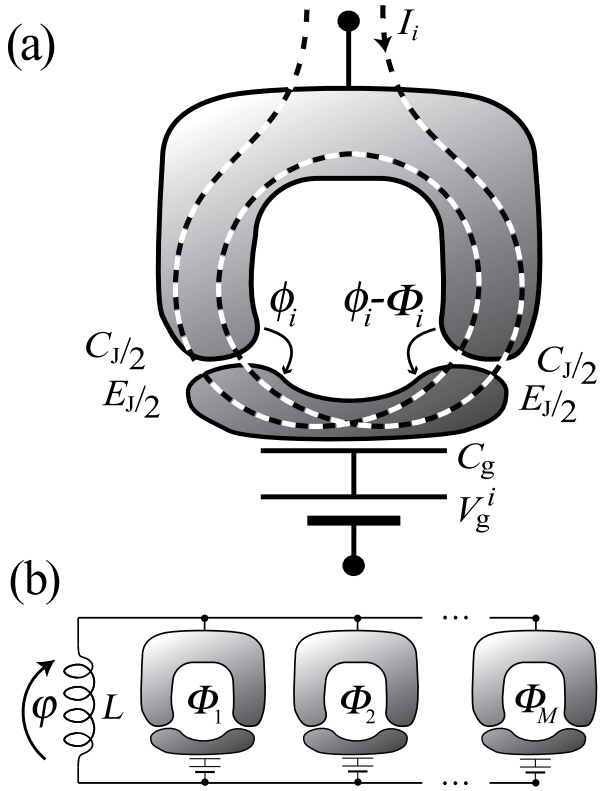

Figure 2. (a) Single Cooper pair box coupled to the environment through a SQUID. (b) Array of Josephson charge qubits coupled inductively.

$2e/\hbar$. The potential energy stored in the junction is $-E_{\rm J}\cos\phi$, where $E_{\rm J}$ is the so-called Josephson energy. Classically, the current flowing through a "large" Josephson junction is $I_{\rm c}\sin\phi$ where I_c is called the critical current and ϕ obeys $\dot{\phi} = 2eV/\hbar$, where V is the voltage. The critical current is related to the Josephson energy via $I_{\rm c} = (2e/\hbar)E_{\rm J}$. SQUIDs are used as tunable Josephson junctions. In the case of identical junctions the Josephson energy term is $-E_{\rm J}\cos(\pi\Phi/\Phi_0)\cos(\phi)$, where $E_{\rm J}/2$ is the Josephson energy of an individual junction, $\Phi_0 = h/2e$ is the flux quantum and Φ is the externally applied flux through the SQUID loop. The normal-state tunneling resistance $R_{\rm T}$ yields the value of $E_{\rm J}$ through the Ambegaokar-Baratoff formula [71] $E_{\rm J} = h\Delta_{\rm BCS}/8e^2R_{\rm T}$, where $\Delta_{\rm BCS}$ is the superconducting gap at zero temperature. A Josephson junction has also a parallel-plate capacitance ($C_{\rm J}/2$ in this case) associated with it, which is typically on the order of fF. The superconducting island is further coupled to a gate voltage $V_{\rm g}$ through a gate capacitance $C_{\rm g}$. These capacitances give rise to a typical charging energy for Cooper pairs $E_{\rm C} = 2e^2/C_\Sigma$, where $C_\Sigma = C_{\rm J} + C_{\rm g}$ is the total capacitance of the island. This charging energy is assumed to be so large that the addition of a single Cooper pair to the island requires more energy than the thermal motion of the environment, roughly speaking, may provide. For charge qubits, we also require that $E_{\rm J} < E_{\rm C}$.

An individual qubit may be manipulated both through the magnetic flux Φ and the gate voltage $V_{\rm g}$. The logical states of the qubit correspond to zero and one extra Cooper pair residing on the island, denoted by $|0\rangle$ and $|1\rangle$ respectively. Since changing the polarization of the island does not induce any tunneling amplitude but, in contrast, changes the relative energy of different charge configurations, the diagonal part of the

two-by-two Hamiltonian for the qubit is controlled through $V_{\rm g}$. However, since the superconducting phase on the island is conjugate to the number of Cooper pairs on the island, it follows that $\cos(\phi)$ gives rise to tunneling and thus the magnetic flux controls the off-diagonal part of the Hamiltonian. Furthermore, Fig. 2(b) illustrates a potential coupling scheme for the charge qubits in which the boxes are fabricated in parallel with an inductance L, possibly realized in practice using a large Josephson junction. The inductor along with the total capacitance of the array of qubits serves as an LC-oscillator whose presence effectively couples the qubits assuming that the frequency of oscillation is much higher than the relevant frequencies of the individual qubits. We may write the Hamiltonian for M qubits (see Paper V and Ref. [25]) as

$$\mathcal{H}_{\rm qb} = \sum_{i=1}^{M} \left[-\frac{B_z^i}{2}\sigma_z^i - \frac{B_x^i}{2}\sigma_x^i \right] - D \sum_{i=1}^{M} \sum_{j=i+1}^{M} B_x^i B_x^j \sigma_y^i \otimes \sigma_y^j \ , \tag{30}$$

where $B_z^i = E_{\rm C}(1-2n_{\rm g}^i)$, $B_x^i = E_{\rm J}(\Phi_i)$ and $D = L(\pi C_{\rm qb}/C_{\rm J}\Phi_0)^2$. We have further denoted $C_{\rm qb} = C_{\rm J}C_{\rm g}/(C_{\rm J}+C_{\rm g})$. The index i refers to the i^{th} qubit. Above $E_{\rm J}(\Phi_i) = E_{\rm J}\cos(\pi\Phi_i/\Phi_0)$ is the effective Josephson energy and $n_{\rm g}^i = C_{\rm g}V_{\rm g}^i$ is the gate charge. It is worthwhile to note that this Hamiltonian is only valid near $n_{\rm g} = 0.5$, i.e. one of the degeneracy points and if $E_{\rm J} \ll E_{\rm C}$. A particularly convenient property of Eq. (30) is that the entire Hamiltonian may be set equal to zero, thereby stopping all temporal evolution. Note that if any two qubits have a non-vanishing tunneling amplitude, they will be automatically coupled. It is easy to construct any single-qubit gate within this model on qubit j by setting $B_x^i = B_z^i = 0$ for $i \neq j$ and by manipulating B_x^j and B_z^j, see Paper V. Using arbitrary one-qubit operations along with almost any nontrivial two-qubit gate [46] one may construct any multiqubit operation. This would not, however, by any means lead to an optimal implementation.

Optimization

In Publication III, the general problem of finding multiqubit gates for the present Hamiltonian is considered. The concept is further developed in Publication IV where particular attention is paid to accelerating algorithms using three-qubit gates. Paper V considers, as an example, the execution of Shor's algorithm on Josephson charge qubits using the optimization method. Just like within HQC, it is possible to associate a loop in the parameter space with every unitary operation. The parameter vector for a k-qubit operation now assumes the form

$$\mathbf{q}(t) = \left[B_z^1(t) \ldots \quad B_z^k(t) \quad B_x^1(t) \quad \ldots \quad B_x^k(t) \right]^T . \tag{31}$$

We may take the origin, where $\mathcal{H}_{\rm qb} = 0$, as the starting point for all quantum-control operations. Then, exactly like in the case of HQC, we may assume that the operations are polygons in the parameter space. Only now the natural parameterization for loops is given by time, and also the speed at which the loops are traversed of course matters. However, we may fix the duration of each edge of the polygon and thus a polygon for k qubits and with $l+1$ vertices has $2l \times k$ degrees of freedom. It is reasonable to require

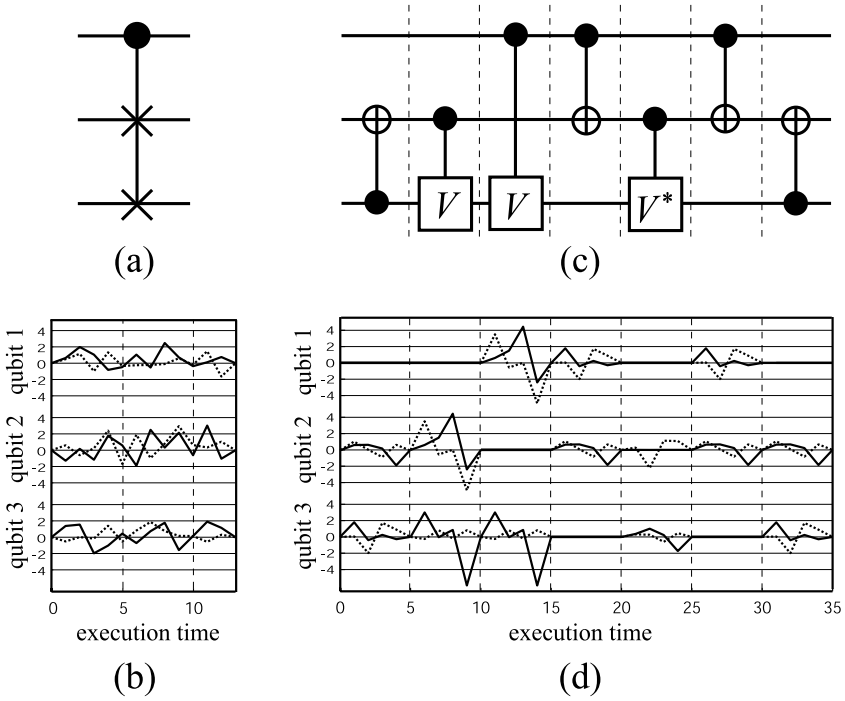

Figure 3. Illustration of the strength of the method in the case of the Fredkin gate. In (a) and (c), the quantum-circuit notation (see text) for the single-shot and decomposed Fredkin gate is shown. Subfigures (b) and (d) show the corresponding parameter pulses. The solid line represents B_z^i while the dashed line represents B_x^i. The resulting direct three-qubit implementation is in this case almost three times faster.

that $2lk \geq 2^{2k} - 1$ in order to achieve[1] the whole $SU(2^k)$. The gates are again found by minimizing $f(\gamma)$ but now the evaluation of U_γ is carried out by discretizing the loop γ into a finite set of points $\gamma_1, \ldots, \gamma_n$ (typically $n = 10^2$–10^4) in the $2k$-dimensional space and since the total time is fixed, we also can fix the time difference Δt between the points and write

$$U_\gamma \approx \exp(-i\mathcal{H}_{\rm qb}(\gamma_n)\Delta t) \ldots \exp(-i\mathcal{H}_{\rm qb}(\gamma_1)\Delta t). \tag{32}$$

It is easy to see from the above expression that one can readily divide the evaluation of the unitary operation into smaller sections of the full loop γ and delegate each subtask to a separate processor. Thus the evaluation of U_γ is almost trivially parallelized, which allows for very efficient optimization. In the case of three-qubit gates, 13 processors were used such that one processor was the master taking care of the optimization routine and the multiplication of the intermediate results was handled by the slaves consisting of the 12 other processors. The length of each linear edge is fixed to one unit and also $D = 1$ as well as $\hbar = 1$. The three-qubit gates require 12 edges and the two-qubit gates call for 5 edges. The results are applicable independent of the sample parameters since rescaling D is possible by simultaneously scaling energy and time.

Figure 3 (Fig. 2 of Paper IV) contains an illustration of the strength of the present

[1]We cannot achieve $U(2^k)$ with the present Hamiltonian since it has been chosen to be traceless, but the global phase is meaningless.

scenario; instead of using the two-qubit gate decomposition of Fig. 3(c) and Fig. 3(d), in which the realization of individual gates has already been optimized, one may search for a minimum of $f(\gamma)$ directly for the whole so-called three-qubit Toffoli gate (see e.g. Ref. [2]). In Fig. 3 as well as in Publications III–V the so-called quantum-circuit notation is used. In this notation, time runs from the left to the right and the horizontal lines represent the history of actions on a particular qubit. In Fig. 3, the qubits are labeled 1, 2 and 3 from top to bottom. A black circle is used to indicate a controlled operation. In Fig. 3(a), for instance, the notation means that a SWAP (denoted by two crosses) is performed between the quantum states of qubits 2 and 3 if the state of the qubit 1 is $|1\rangle$. Otherwise nothing is done. This is in fact the definition of the Toffoli gate. In Fig. 3(c), on the other hand, a sequence of seven operations performing the Toffoli gate in seven substeps is illustrated. The first (leftmost) operation is a controlled-NOT (CNOT) which flips the qubit 2 iff the qubit 3 is $|1\rangle$. The controlled-V operation means that the operation $V = \sqrt{\sigma_x}$ is carried out iff the control qubit is $|1\rangle$. Furthermore, the star in Fig. 3(c) stands for a Hermitean conjugate. A matrix representation can of course be used for any gates provided that an ordering of the subsystems, i.e. the vector presentation, has been fixed, but the quantum circuit notation is in many ways much more informative. For more on this notation see e.g. Ref. [2].

It should be clear from Fig. 3 why the direct implementation is superior. Instead of allowing one qubit to be idle (parameters B_x^i and B_z^i set to zero) we can operate on all the three qubits simultaneously. The resulting single-shot pulse sequence is almost three times faster than the decomposed version. More examples of optimized gates may be found in Publications III–V.

Alternative: Optimal control theory

It is also possible to apply tools from optimal control theory (OCT) in the design of control pulses for Josephson qubits. Figure 4 illustrates a control pulse for the three-qubit Fourier transform that was calculated using an algorithm complementary to ours described recently in Refs. [72, 73] along with a pulse obtained using our method. This method is somewhat different from the method presented in this Thesis and relies on the use of variational calculus. Both methods, OCT and the polytope search, scale exponentially with the number of qubits. Both methods can be parallelized too. The OCT algorithm, however, yields a smooth control pulse, but it would also be possible to use smooth pulses with our method as well. Then the node degrees of freedom would be replaced, for instance, by the coefficients of some basis functions. In both OCT and our approach it is possible to take into account the limitations of a particular experimental situation and design the control pulses accordingly. Thus, the piecewise linear pulses presented in this Thesis should be considered merely as examples. Nevertheless, the philosophy of our method and the OCT in the context of quantum computing is the same; in both cases the use of elementary gates can be avoided and the execution time and errors decreased. Comparing the relative superiority of our method and OCT would call for a separate study and the results would probably depend strongly on the exact form of the Hamiltonian.

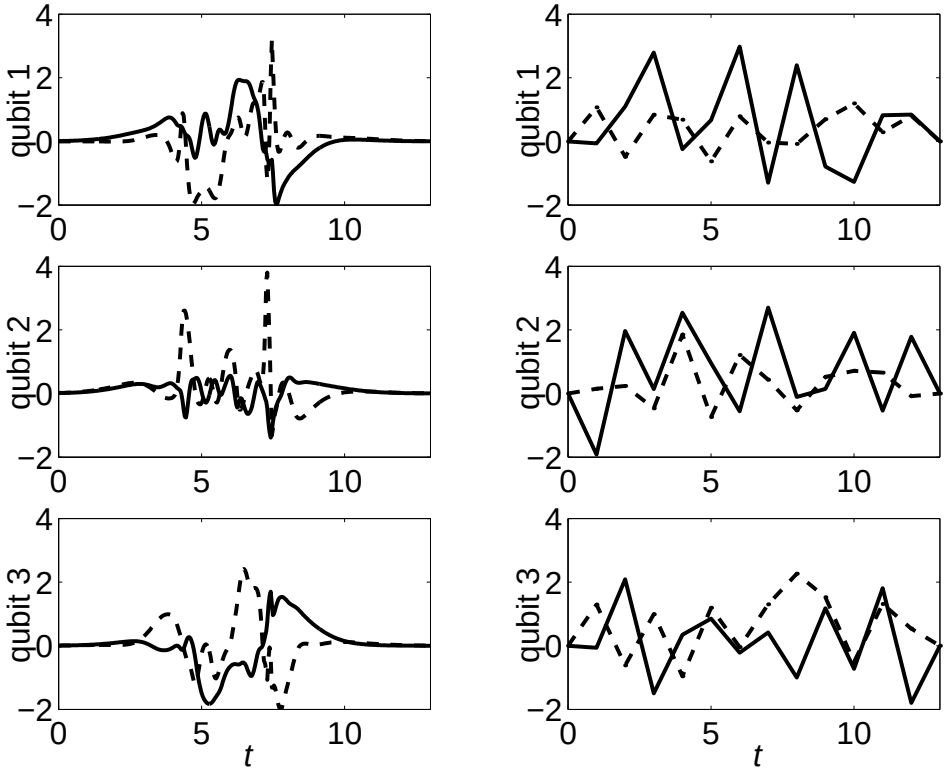

Figure 4. (left) An optimal control theory realization of the quantum Fourier transform for three qubits. The dashed line indicates B_x^i and the solid line represents B_z^i. (right) Piecewise linear realization of the QFT from Paper III.

Example: Factoring 21

Publication V discusses the feasibility of factoring the number 21 using the numerical optimization method developed here using inductively coupled Josephson qubits. The number 21 is arguably the smallest nontrivial number[2] to be factored using Shor's algorithm. Figure 5 of this Paper illustrates the full quantum circuit for the quantum part of the algorithm. As many as 5900 two-qubit gates and 2300 three-qubit gates are involved in the implementation. If only (arbitrary) two-qubit qubit gates were available, then some 16 400 of them would be required. The number of elementary gates would be necessarily orders of magnitude higher, depending on the exact set available. However, in any realistic scenario the use of a limited set of elementary gates is not viable; every measure of cutting down the execution time of the quantum part of the algorithm needs to be taken. Thus even very heavy classical preoptimization is justifiable. Nevertheless, for a superconducting Al sample the runtime of the algorithm would at best be 10^{-6} s. This coincides with the best experimental estimates for the coherence time of a superconducting system [22], though for only a single qubit at a special point. The use of arbitrary two-qubit gates instead of three-qubit gates would increase the runtime by some 40%. The number of required qubits would be 22 with two independent controls per qubit. Clearly this kind of an experiment with the requirement that the tempera-

[2]The first obvious choice would be 15 but in this case the classical preprocessing happens to reveal the answer, see Publication V. Of course $21 = 3 \times 7$, but this is not a triviality of the same kind.

ture of the environment be around tens of mK is not easy and would probably require dedicated low-temperature control circuitry, such as rapid single flux quantum (RSFQ) logic [74,75]. Otherwise at least 44 RF-lines and very complicated pulse generators would be mandatory. Despite the difficulties, factoring 21 on superconducting qubits should be possible with very careful design.

Using a scaling argument we may also comment on the factoring of numbers large enough to break the RSA cryptosystem in the absence of any active coherence preservation method, such as error correction [2, 76]. For instance, breaking the 512-bit RSA would require thousands of qubits and since the runtime scales at best as $n^3 \log n$, where n is the number of bits it takes to represent the number to be factored, we can argue based on the estimates given above that tens of seconds of decoherence time is necessary. The number of independent high-frequency controls would be thousands. Clearly a scalable implementation of a superconducting quantum computer is extremely challenging and far in the future. However, many applications rely on very similar ideas and these are quite reachable even today. One such application is considered in the next Section.

4 Cooper Pair Pumping

In this Section we consider an application of Berry's [31] Abelian geometrical phase to Cooper pair pumping using mesoscopic Josephson junctions. Particular attention is paid to the so-called Cooper pair "sluice" introduced in Paper VI. The idea of operation and the techniques used are very similar to the control of Josephson charge qubits. Actually, a Cooper pair "sluice" in a proper environment could serve as a qubit, since the Hamiltonian presented below offers more than enough possibilities for control. Mastering the flux and voltage control of only a few superconducting qubits, which is being pursued by many groups worldwide, does not necessarily have immediate practical impact in the field of quantum computing. However, spin-offs such the "sluice" may find uses, e.g., in metrology. Some differences between Cooper pair pumping and superconducting qubits exist, though. For instance, superpositions of energetically different states are not pursued and the basic control pulse (pumping cycle) is applied repetitively in contrast to single-shot quantum gates.

As to charge pumps in general, a seven-junction single-electron pump [30] with currents on the order of pA has been demonstrated to be usable as a capacitance standard [77], but the realization of the so-called quantum metrological triangle [78] would require currents on the order of nA. This is beyond single-electron pumps, but Cooper pair pumps could potentially yield currents accurately in the nA range. The use of Surface Acoustic Waves (SAW) to pump electrons is being studied actively as an alternative to ordinary electron pumps, see e.g. Ref. [79]. The engineering of the electromagnetic environment of both electron pumps [80] as well as Cooper pair devices [81] using on-chip resistors has been considered in order to achieve a frequency-locked current source. No metrological Cooper pair pump has been realized yet.

The considered form of the temporal control is not found numerically but rather using analytic physical arguments. In Subsection 4.1, the relationship between Cooper pair pumping and Berry's phase is discussed. Subsection 4.2 discusses the theory of the "sluice". Subsection 4.3, based on the experiments of Publication VII, is the highlight of the present Section.

4.1 Adiabatic Cooper pair pumping and Berry's phase

An adiabatic Cooper pair pump is a chain of Josephson junctions with at least two tunable parameters. For instance the first measured pump of Geerligs et al. [26] had three Josephson junctions in a chain and two voltage gates coupled to the islands in between. A similar structure was also recently measured by Toppari et al. [82]. However, longer chains, including the seven-junction Cooper pair pump of Aumentado et al. [83], have been studied as well. The requirement that at least two parameters are needed is due to the fact that the pumping effect is attributable to a loop in the parameter space. We will make the connection between the pumped charge and Berry's phase clear in simple terms. For a more formal derivation see Ref. [84].

The Cooper pair pump shown in Fig. 5 serves as a generic model that encompasses both the traditional gate-controlled pumps and the flux-assisted pump studied here. For

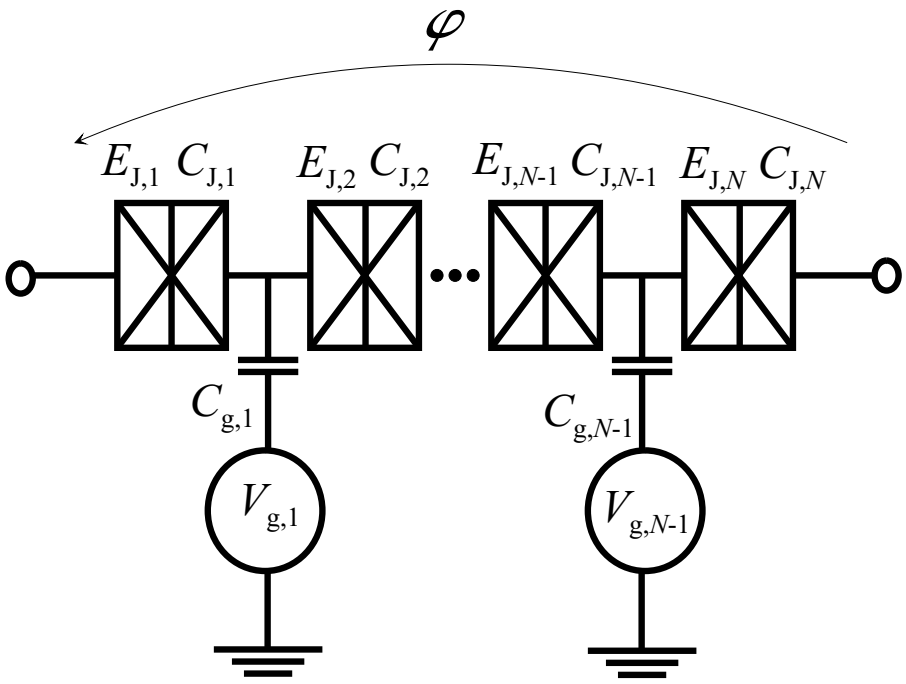

Figure 5. Generic model of a Cooper pair pump.

now, the device is assumed to be phase biased such that the superconducting phase difference over the device is φ. The average current operator for a chain of Josephson junctions is given by

$$\mathcal{I} = \frac{2e}{\hbar}\frac{\partial \mathcal{H}_{\mathrm{pump}}}{\partial \varphi}. \tag{33}$$

Assuming, for simplicity, that $C_{\mathrm{J},j} = C_{\mathrm{J}}$ for all j and that $C_{\mathrm{g},j}/C_{\mathrm{J}} \ll 1$ allows us to write the Hamiltonian for an N-junction pump in the absence of quasiparticles as

$$\begin{aligned}\mathcal{H}_{\mathrm{pump}} = \frac{1}{2}(\hat{\mathbf{n}} - \mathbf{n}_{\mathrm{g}})^{\mathrm{T}}\mathbb{C}^{-1}(\hat{\mathbf{n}} - \mathbf{n}_{\mathrm{g}}) - \sum_{k=2}^{N-1} E_{\mathrm{J},k}\cos(\phi_{k-1} - \phi_k + \varphi/N) \\ - E_{\mathrm{J},1}\cos(\varphi/N - \phi_1) - E_{\mathrm{J},N}\cos(\varphi/N + \phi_{N-1}).\end{aligned} \tag{34}$$

Here $E_{\mathrm{J},k}$ is the Josephson energy of the k^{th} junction and ϕ_k is the superconducting phase on the k^{th} island whereas $\mathbb{C}$ is the three-band capacitance matrix of the junction chain given by

$$\mathbb{C} = \begin{pmatrix} C_{\mathrm{g},1} + 2C_{\mathrm{J}} & -C_{\mathrm{J}} & & \\ -C_{\mathrm{J}} & C_{\mathrm{g}} + 2C_{\mathrm{J}} & -C_{\mathrm{J}} & \\ & \ddots & \ddots & \\ & & -C_{\mathrm{J}} & C_{\mathrm{g},N-1} + 2C_{\mathrm{J}} \end{pmatrix}. \tag{35}$$

Allowing the Josephson energies to be different for each junction, even though the capacitances are equal, anticipates the developments of the next Subsection. The number operators of Cooper pairs $\hat{n}_k$ of each of the islands and the gate charges $n_{\mathrm{g},k} = C_{\mathrm{g},k}V_{\mathrm{g},k}$

are contained in $\hat{\mathbf{n}}$ and $\mathbf{n}_{\mathrm{g}}$, that is

$$\hat{\mathbf{n}} = \begin{pmatrix} \hat{n}_1 \\ \vdots \\ \hat{n}_N \end{pmatrix} \qquad \text{and} \qquad \mathbf{n}_{\mathrm{g}} = \begin{pmatrix} n_{\mathrm{g},1} \\ \vdots \\ n_{\mathrm{g},N} \end{pmatrix}. \tag{36}$$

Now let us assume that the parameters of the system denoted collectively by $\mathbf{q}(t)$ are tuned adiabatically around a cycle γ in the parameter space over the time $t \in [0, t_{\mathrm{cycle}}]$ and that the ground state is non-degenerate. What the parameters are is not important for the derivation. Clearly, the total charge that passes through the device is

$$Q_{\mathrm{tot}} = \int_0^{t_{\mathrm{cycle}}} \langle \psi(t)|\mathcal{I}|\psi(t)\rangle dt, \tag{37}$$

where $|\psi(t)\rangle$ is the state vector of the pump at the time t. Using Eq. (9) of Section 2 with $g = 1$ as well as Eq. (11) allows us to write the state of the pump at time t as

$$|\psi(t)\rangle = e^{i\theta(t)}|0;\mathbf{q}(t)\rangle \tag{38}$$

due to the adiabaticity assumption. Here $|0;\mathbf{q}\rangle$ is the ground-state vector which depends on the control-parameter vector $\mathbf{q}$. The phase $\theta(t)$ has two contributions, namely the dynamical phase

$$\theta_{\mathrm{dyn}}(t) = -\frac{1}{\hbar}\int_0^t \langle 0;\mathbf{q}(\tau)|\mathcal{H}_{\mathrm{pump}}|0;\mathbf{q}(\tau)\rangle d\tau \tag{39}$$

and the geometrical phase

$$\theta_{\mathrm{geom}}(t) = i\int_0^t \langle 0;\mathbf{q}(\tau)|\frac{d}{d\tau}|0;\mathbf{q}(\tau)\rangle d\tau = i\int_{\mathbf{q}(0)}^{\mathbf{q}(t)} \langle 0;\mathbf{q}|\nabla_{\mathbf{q}}|0;\mathbf{q}\rangle \cdot d\mathbf{q}. \tag{40}$$

At time t_{cycle} it holds in particular that

$$\theta_{\mathrm{Berry}} \equiv \theta_{\mathrm{geom}}(t_{\mathrm{cycle}}) = i\oint_\gamma \langle 0;\mathbf{q}|\nabla_{\mathbf{q}}|0;\mathbf{q}\rangle \cdot d\mathbf{q} \tag{41}$$

since at this instant the cycle is full. Now, it is possible to rewrite the integrand in Eq. (37) as

$$\langle \psi(t)|\mathcal{I}|\psi(t)\rangle = \langle \psi(t)|\frac{2e}{\hbar}\frac{\partial \mathcal{H}_{\mathrm{pump}}}{\partial \varphi}|\psi(t)\rangle = \frac{2e}{\hbar}\langle \psi(t)|\left[\frac{\partial}{\partial \varphi}, \mathcal{H}_{\mathrm{pump}}\right]|\psi(t)\rangle. \tag{42}$$

Owing to the Schrödinger equation, we may further write

$$\langle \psi(t)|\mathcal{I}|\psi(t)\rangle = 2ei\frac{d}{dt}\left(\langle \psi(t)|\frac{\partial}{\partial \varphi}|\psi(t)\rangle\right). \tag{43}$$

On the other hand

$$\begin{aligned} \langle \psi(t)|\frac{\partial}{\partial \varphi}|\psi(t)\rangle &= \langle 0;\mathbf{q}(t)|e^{-i\theta(t)}\frac{\partial}{\partial \varphi}e^{i\theta(t)}|0;\mathbf{q}(t)\rangle \\ &= i\frac{\partial \theta(t)}{\partial \varphi}\langle 0;\mathbf{q}(t)|0;\mathbf{q}(t)\rangle + \langle 0;\mathbf{q}(t)|\frac{\partial}{\partial \varphi}|0;\mathbf{q}(t)\rangle \\ &= i\frac{\partial \theta(t)}{\partial \varphi} + \langle 0;\mathbf{q}(t)|\frac{\partial}{\partial \varphi}|0;\mathbf{q}(t)\rangle. \end{aligned} \tag{44}$$

The pumped charge is thus (use $\mathbf{q}(0) = \mathbf{q}(t_{\rm cycle})$ and $\theta(0) = 0$)

$$Q_{\rm tot} = -2e \int_0^{t_{\rm cycle}} \frac{d}{dt}\left(\frac{\partial\theta(t)}{\partial\varphi}\right) dt + \underbrace{\int_0^{t_{\rm cycle}} 2ei\frac{d}{dt}\langle 0;\mathbf{q}(t)|\frac{\partial}{\partial\varphi}|0;\mathbf{q}(t)\rangle dt}_{=0}$$
$$= -2e\frac{\partial}{\partial\varphi}\left(\theta_{\rm dyn}(t_{\rm cycle}) + \theta_{\rm Berry}\right). \tag{45}$$

The total charge transferred is $-2e$ times the derivative of the phase accumulated over one cycle with respect to the global superconducting phase difference. The first part, or the dynamical contribution is

$$Q_{\rm s} = -2e\frac{\partial}{\partial\varphi}\left(\theta_{\rm dyn}(t_{\rm cycle})\right) = \frac{2e}{\hbar}\frac{\partial}{\partial\varphi}\int_0^{t_{\rm cycle}} \langle 0;\mathbf{q}(t)|\mathcal{H}_{\rm pump}|0;\mathbf{q}(t)\rangle dt$$
$$= \int_0^{t_{\rm cycle}} \langle 0;\mathbf{q}(t)|\mathcal{I}|0;\mathbf{q}(t)\rangle dt \tag{46}$$

which is just the "classical" Josephson supercurrent. In pumping applications one tries to suppress the supercurrent altogether. The second contribution is the more nontrivial pumped charge

$$Q_{\rm p} = -2e\frac{\partial}{\partial\varphi}\left(\theta_{\rm Berry}\right) = -2e\frac{\partial}{\partial\varphi}\oint_\gamma i\langle 0;\mathbf{q}(t)|\nabla_{\mathbf{q}}|0;\mathbf{q}(t)\rangle\cdot d\mathbf{q} \tag{47}$$

and as may be seen, this is in close connection with Berry's phase. Thus pumping Cooper pairs may, very naturally, be seen as an observable manifestation of Berry's phase. It is remarkable that Berry's phase of a nondegenerate ground state has observable consequences while for instance in quantum computing either degeneracy (holonomy) or superpositions of energetically different states are required for observable consequences. In quantum computing the loop γ applies a logical operation whereas here it pumps charge.

It is possible to derive from Eq. (47) a more elaborate expression for the pumped charge appearing often in literature. We may write

$$Q_{\rm p} = 2\hbar\,{\rm Im}\left[\sum_{m=1}^{\infty}\oint_\gamma \frac{\langle 0;\mathbf{q}|\mathcal{I}|m;\mathbf{q}\rangle}{\varepsilon_{\mathbf{q},0} - \varepsilon_{\mathbf{q},m}}\langle m;\mathbf{q}|\nabla_{\mathbf{q}}|0;\mathbf{q}\rangle\cdot d\mathbf{q}\right], \tag{48}$$

where $|m;\mathbf{q}\rangle$ is the $m^{\rm th}$ energy eigenstate and $\varepsilon_{\mathbf{q},m}$ is its energy. This is the form found first in Ref. [27] and the equivalence between Eq. (48) and Eq. (47) is demonstrated in Ref. [84].

4.2 Cooper pair "sluice"

The expressions derived above for the pumped charge are quite general and the exact nature of the tunable parameters has not yet been specified. Traditionally, charge pumping through a chain of Josephson junctions is achieved via cyclically manipulating gate voltages in such a manner that the state of the system propagates adiabatically through

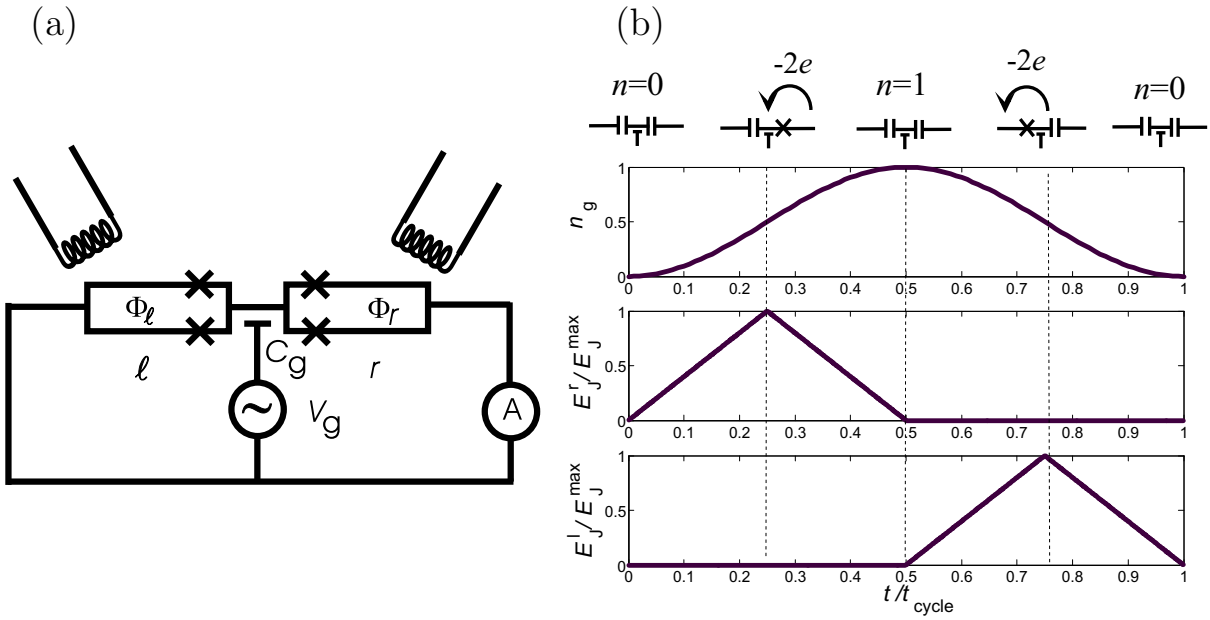

Figure 6. (a) Schematic of the Cooper pair "sluice". (b) Pulse sequence for pumping a single Cooper pair through the sluice. The exact form of the pulses is not crucial as long as synchronization is maintained.

a series of near-eigenstates of charge. For instance, in the three-junction Cooper pair pump [26, 27, 82] one may denote by (Q_1, Q_2) the eigenstate of charge with Q_1 residing on island 1 and Q_2 residing on island 2. Then the gate voltages are manipulated adiabatically such that the cycle $(Q_1, Q_2) : (0, 0) \to (0, 2e) \to (2e, 0) \to (0, 0)$ is almost achieved. However, due to the non-vanishing Josephson coupling, the eigenstate of energy is not an eigenstate of charge. It is impossible to decrease the Josephson energies of the junctions indefinitely without sacrificing the adiabaticity since the smallest excitation energy is proportional to E_J. Stated otherwise, there is a tradeoff between accuracy and adiabaticity. From the point of view of adiabaticity it would be beneficial to increase E_J indefinitely, but in the adiabatic limit there is an error in the pumped charge proportional to E_J such that it would be desirable to make E_J small. These two seemingly contradicting requirements are the reason for considering tunable Josephson junctions, i.e. SQUIDs.

The Cooper pair sluice is a single-island Cooper pair pump. It was introduced and analyzed theoretically in Publication VI. A single island and a single gate voltage are sufficient due to the fact that also the couplings are controlled. A schematic of the device is shown in Fig. 6(a). The Hamiltonian of a homogeneous Cooper pair sluice is explicitly

$$\begin{aligned}\mathcal{H}_\mathrm{sluice} =& E_\mathrm{C}(\hat{n} - n_\mathrm{g})^2 - E_\mathrm{J}^\mathrm{r}\left(\pi\frac{\Phi_\mathrm{r}}{\Phi_0}\right)\cos(\phi + \varphi/2) \\ & - E_\mathrm{J}^\mathrm{l}\left(\pi\frac{\Phi_\mathrm{l}}{\Phi_0}\right)\cos(\varphi/2 - \phi). \end{aligned} \tag{49}$$

Here ϕ is the phase on the island and $\hat{n}$ is the number operator for Cooper pairs. They obey the commutation relation $[\hat{n}, \phi] = i$. The charging energy is given by

$E_{\rm C} = 2e^2/(2C_{\rm J} + C_{\rm g})$ and the gate charge is $n_{\rm g} = C_{\rm g}V_{\rm g}/2e$. Furthermore, $E_{\rm J}^{\rm l}$ and $E_{\rm J}^{\rm r}$ are the effective Josephson energies of the left and right SQUIDs, respectively, which we assume may in principle be set to zero. The flux through the left (right) junction is denoted by $\Phi_{\rm l}$ ($\Phi_{\rm r}$). The parameter vector $\mathbf{q}$ for the present device is given by $\mathbf{q} = (n_{\rm g}, E_{\rm J}^{\rm r}, E_{\rm J}^{\rm l})^{\rm T}$. The pumping of charge is achieved via manipulating the parameters $\mathbf{q}$ adiabatically such that at certain instants the ground state is ideally also exactly an eigenstate of charge. This may be achieved by setting the Josephson couplings to zero. A typical pumping cycle is shown in Fig. 6(b).

For instance, we may assume that initially the ground state is an eigenstate with zero Cooper pairs which we attain e.g. with $E_{\rm J}^{\rm l} = 0$, $E_{\rm J}^{\rm r} = 0$ and $n_{\rm g} = 0$. Then keeping $E_{\rm J}^{\rm r} = 0$ and tuning $n_{\rm g}$ from zero to one and simultaneously opening the left SQUID (first vertical dashed line in Fig. 6(b)) and closing it again (second dashed line) adiabatically increases the number of Cooper pairs on the island by one. Namely, the ground state is after the manipulation still an eigenstate of charge but with one more pair and we have assumed that the system stays at its ground state. The extra Cooper pair must have tunneled through the left SQUID since the right one was closed altogether. Ramping $n_{\rm g}$ from one again back to zero while simultaneously opening (third dashed line) and closing the right SQUID clearly takes us to where we began: The island again has zero Cooper pairs. This time the charge must have flown through the left SQUID. In conclusion, this cycle leads to a pumping of exactly one Cooper pair through the device. Repeating the cycle at the frequency f leads to a DC current $I = 2ef$. Note that the above logic immediately generalizes to the pumping of m Cooper pairs by working between $n_{\rm g} = 0$ and $n_{\rm g} = m$ yielding $I = 2emf$. The crucial assumption is that the temporal evolution is adiabatic. It is worth pointing out explicitly that the above cycle maintains the non-degeneracy of the ground state such that the system indeed is protected against excitations to higher levels.

The imperfections of the sluice have been analyzed in Publication VI. To this end, the sluice was simulated using numerical integration of the Schrödinger equation. This was carried out using the loop shown in Fig. 6(b) as a basis for the time dependence of the Hamiltonian $\mathcal{H}_{\rm sluice}$. Then, just like in the case of quantum algorithms, the time axis was split to a discrete set of points (10^6 or more) that were a distance Δt apart and the Hamiltonian was considered piecewise constant in time. The Hilbert space was truncated to some 10–30 charge states depending on the value of m considered. The state vectors were propagated using

$$|\psi(t + \Delta t)\rangle \approx \exp(-i\mathcal{H}_{\rm sluice}(t + \Delta t/2)\Delta t/\hbar)|\psi(t)\rangle. \tag{50}$$

The quantity of interest, $Q_{\rm P}$ in Eq. (37) was evaluated simply using the trapezoidal rule. Note that the current operator also has a time dependence. The discretization was made fine enough such that increasing the number of points did not change the result.

It was found that the pumping of individual Cooper pairs with an accuracy of 10^{-7} should be possible at currents of some 10 pA. However, increasing m to $m = 10$, would allow pumping of 0.1 nA with the same accuracy. These estimates only take into account the finite operating frequency. The optimal value of m is not known. It was

also found that with sufficient phase averaging errors should not increase. Namely, the leakage supercurrent is proportional to $\sin\varphi$ while the error in the pumped charge $Q_{\rm P}$ is proportional to $\cos\varphi$. The average of both of these under a perfect voltage bias V is clearly zero since then $\varphi = 2eVt/\hbar$.

4.3 Experiments on the "sluice"

Paper VII describes the experiments demonstrating the pumping of Cooper pairs utilizing the idea described above. Figure 7 shows scanning electron micrographs (SEM) of the measured sample as well as a schematic of the measurement setup. The sample was fabricated using standard e-beam lithography and two-angle shadow evaporation. The steps of the fabrication process included spinning a two-layer PMMA/MAA (polymethyl methacrylate/methacrylic acid) and PMMA resist on top of a silicon wafer, drawing the pattern of the device using an electron beam, developing the resist in two different solvents (first in a mixture of 25% MIBK (methyl isobutyl ketone) and 75% IPA (isopropanol) and then in pure IPA) to get an "undercut" and finally evaporating aluminum from two different angles in vacuum with an oxidization step between the layers. The Josephson junctions are thus realized as an Al-AlO_x-Al sandwich. The thicknesses of the Al layers were 30 nm and 50 nm while the thickness of the oxide is a few nm. The extra aluminum was removed in the lift-off done by dipping the chip in acetone. The two different layers can be seen as "shadows" in Fig. 7(b). The sample was then attached to the sample holder of a He^3- He^4 dilution cryostat with a base temperature of 20 mK and electrically connected using Al wire bonds. The two ends of the device were bonded to DC lines in a four-point configuration as shown in Fig. 7(c) while the two input coils and the gate were connected to RF lines with bandwidth up to tens of GHz. The measurement electronics along with the arbitrary waveform generators used for realizing the flux and voltage control were connected to a PC. `Matlab` scripts and `Matlab`'s `Data Acquisition Toolbox` were used to carry out the measurement.

The sample parameters were $C_{\rm g} \approx 0.2$ fF, $E_C/k_{\rm B} \approx 1$ K and $E_{\rm J}/k_{\rm B} \approx 0.5$ K. The estimate of the gate capacitance is based on gate periodicity measurements, that of the charging energy on the measurement of the normal-state conductance at 4.2 K [85] while the estimate of $E_{\rm J}$ is based on the normal-state resistance and the Ambegaokar-Baratoff formula [71], i.e., $E_{\rm J} = h\Delta_{\rm BCS}/8e^2R_{\rm T}$. For the arrangement of the flux pulsing it is important to know the mutual inductances between the input coils and the SQUIDs. The SQUIDs were intentionally designed to have large extensions to get better coupling. The mutual inductances were measured by sweeping the DC current in the two input coils at constant bias voltage and by measuring the current. This allows one to design the flux pulses with proper compensations for the cross-talk, see Publication VII. The relative phases were optimized by sweeping them and maximizing the current. Since we were using commercial waveform generators, we were forced to use frequencies on the order of a few MHz. Luckily, though, we could compensate for the low frequency by increasing the number of pumped charges m, i.e. the gate amplitude.

The measurement of the full current-voltage characteristics was carried out with the

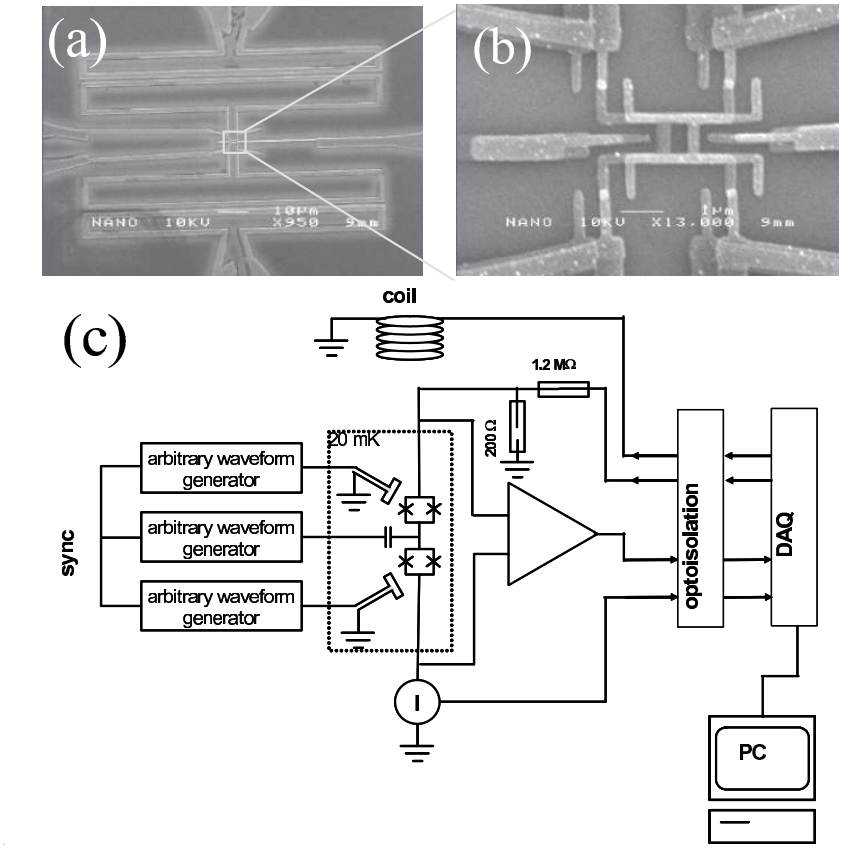

Figure 7. (a) Scanning electron micrograph of the Cooper pair "sluice". The input coils are seen topmost and lowest in the picture while the gate extends to the right. The current flows between the two electrodes on the left. (b) Close-up of the island. The Josephson junctions are the four lighter-shade spots formed in the overlap of the two shadows. (c) Measurement setup.

pumping signal being applied underneath. It was found that despite the manipulation of the Josephson energies, leakage current unfortunately also existed. However, since it was possible to change the direction of the current by shifting the phase of the gate through 180 degrees, it is possible to extract the pumped current from this measurement. Namely, subtracting the IVs with the pumping applied forward and backward from each other should leave us with twice the pumped current. Figure 8 shows full IVs at 3 MHz for different gate amplitudes with pumping in both directions along with the aforementioned differences ΔI vs. voltage. It is seen that the difference in the current nicely obeys the expected pumping behavior. In order to serve as a practical current pump the leakage should be taken care of, e.g., by improved voltage biasing and/or improving the closing of the SQUIDs.

The most convincing evidence of the pumping along with the fact that the above phase shift procedure works, is found by gradually increasing the gate amplitude and then measuring the current at a constant voltage bias. The results are shown in Fig. 9. The quantity that we studied was ΔI in this measurement too. The amplitude was increased such that the low level of the gate $V_{\rm g}^{\rm lo}$ was fixed and the high level $V_{\rm g}^{\rm hi}$ was swept. This

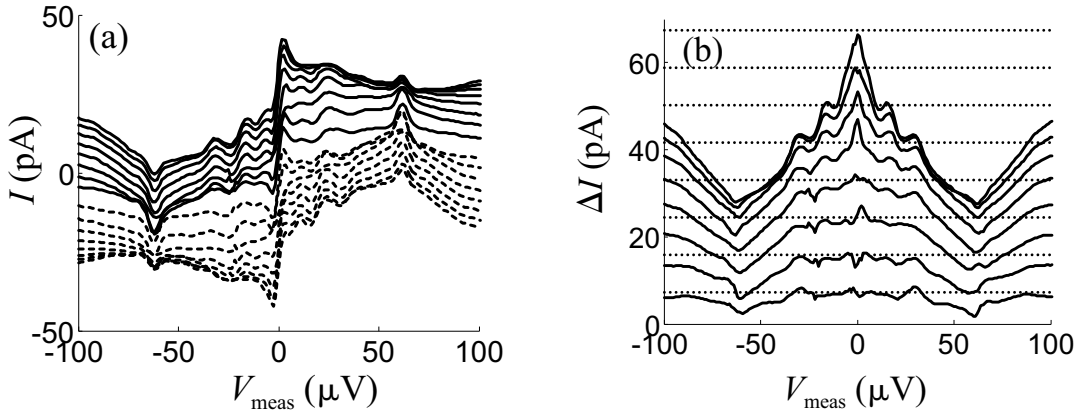

Figure 8. (a) IVs for pumping forward (solid) and backward (dashed). Here m ranges between 4 and 34. (b) Differences ΔI in the IVs (see text). Horizontal dotted lines indicate the expected levels of current. Here $V_{\rm meas}$ is the measured value of voltage.

should result in $2e$-periodic staircase in the pumped current with the step heights[3] equal to $4ef$. However, due to quasiparticle poisoning faster than the measurement time scale but slower than the pumping, the measured behavior was e-periodic with $2ef$ steps. This is interpreted to be because we actually measure the average of two $2e$-periodic staircases shifted by e with respect to each other. Figure 9(b) also shows the high gate amplitude behavior of ΔI and it is seen that up to amplitudes of $10e$ the agreement with the expected behavior is good. Fig. 9(c) illustrates the least-squares fitted slopes to the linear regime of Figs. 9(a–b). The agreement with theory is seen to be good with a few percent error.

To conclude, we have demonstrated in practice the original idea of Publication VI for pumping Cooper pairs with tunable Josephson junctions, i.e. SQUIDs. The experimental evidence is convincing enough to show that the idea for pumping works, although several non-idealities still exist. Possible solutions for cutting down the leakage include fabricating an on-chip capacitor much larger than the junction capacitance parallel with the pump, considering a more complicated design for the SQUIDs (see Fig. 1(b) of Publication VI) and maybe even using a longer array. Lengthening the array would, though, inevitably complicate the control. The capacitance, however, would better conserve the energy of the pump since then the so-called P(E)-curve would be peaked close to the zero of energy, see e.g. Ref. [70]. The quasiparticle poisoning is not necessarily a problem even from the application point of view, if the quasiparticle current is small enough. Namely, our measurements indicate that the net quasiparticle flow is negligible but, instead, the quasiparticles jump randomly on and off the island with no preferred direction. That is, the flow of current is mostly due to Cooper pairs. The quasiparticles in the present measurement are thus probably of the non-equilibrium type reported in Ref. [86]. There the reported time scale of quasiparticle poisoning for a superconducting SET was 10 μs. In Ref. [87] the relevant time-scale was 10^{-2} s but in a somewhat different setup. These figures support our time scale argument, since the integration time for our measurement

[3]Recall that ΔI should be twice the pumped current.

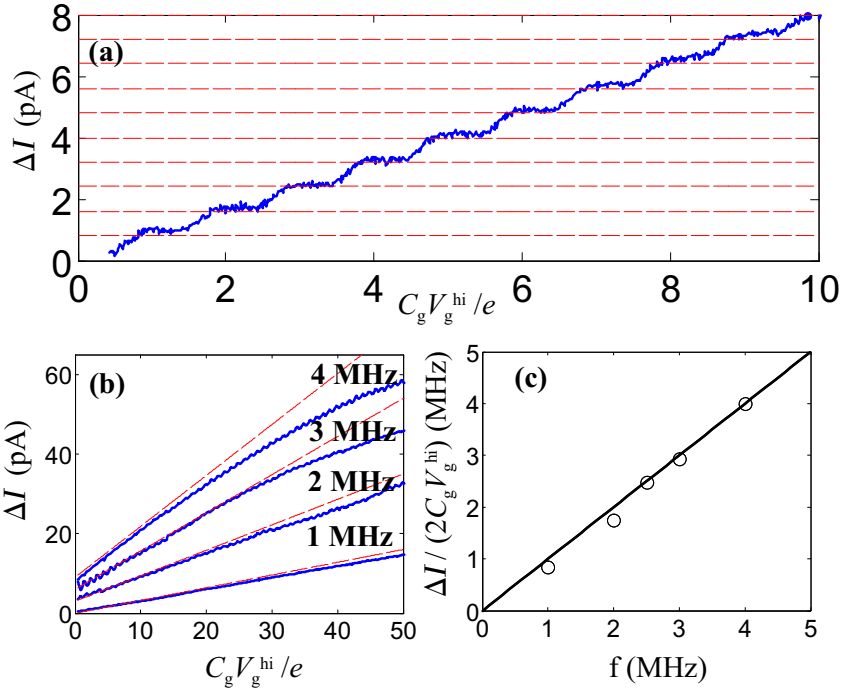

Figure 9. (a) Difference ΔI in the current for forward and backward pumping at 2.5 MHz against the high level of the gate signal V_g^{hi} with the low level at zero. The dashed lines are drawn at $2ef$ intervals. (b) Large gate amplitude behavior of ΔI at a few frequencies. The dashed lines show the expected gate dependence, i.e. their slope is $2ef$. The curves are offset for clarity. (c) Fitted slopes to the data of the previous plots up to $V_g C_g/e = 10$ are shown by circles. The solid line indicates the expected behavior. The voltage bias point was around 10 μV in all the above plots.

was on the order of 0.1 s and the pumping time smaller than 1 μs. We could not, however, experimentally determine the characteristic time for quasiparticles in the present setup.

5 Conclusions

In this Overview we have discussed different aspects of the controlled evolution of quantum systems, both geometrical and dynamical. Particular attention was paid to nanoscale Josephson junction circuits. The two applications that were considered in detail included quantum computing and quantum charge pumping. Let us briefly summarize the conclusion of the Publications included in this Thesis:

In Publications I–II, a realization independent numerical method of finding arbitrary holonomic quantum gates was studied. It was shown that holonomy loops realizing any one and two-qubit unitary operation for the studied three-state model can be found easily. Moreover, it was shown that the length of the loop could be reduced by numerical optimization.

In Publications III–V, the optimization method was generalized to dynamical quantum computing. The physical system studied was the inductively coupled Josephson charge qubit array, although the method could easily be generalized to other systems. The algorithm was parallelized and shown to be capable of finding single-shot realizations for up to three-qubit gates. Publication III introduced the method while Publication IV concentrated on accelerating quantum algorithms using three-qubit gates. The more extended Publication V discussed the requirements of performing Shor's algorithm on the inductively coupled charge-qubit array. It was found that factoring 21, arguably the simplest "non-trivial" composite integer, would require 22 qubits and microsecond coherence times which is on the same order as the best reported coherence times in superconducting circuits. However, it was found, that breaking for instance the 512-bit RSA would require thousands of qubits working co-operatively and tens of seconds in terms of coherence time. All the estimates were based on the assumption that arbitrary three-qubit gates are available in single-shot form. The use of elementary gates would prolong the runtime severely. The conclusion regarding Publications I-V is that even though no change in the complexity of the algorithm is obtained via numerical optimization, the stringent limits set by short decoherence times makes it well worthwhile to try and reduce the runtime even by a numerical factor. Optimization may well result in cutting down the runtime by orders of magnitude opposed to elementary-gate logic inspired by classical computers.

In Publication VI, an application of Berry's geometrical phase in a superconducting circuit was discussed. There a novel Cooper pair pump, the "sluice", consisting of just one superconducting island connected to leads via SQUID loops and utilizing both flux and voltage control was introduced. It was shown that the device can potentially reach metrological accuracy. In Publication VII, the experimental results of the device were reported. It was found that the pumped current increases in clear steps with the increasing gate amplitude and changes direction under a 180-degree phase shift of the gate, even though quasiparticle poisoning and leakage were present. Many suggestions for improving the device were given. The "sluice" was found to be a promising candidate for a practical current pump. The clear benefit of the "sluice" is that it is simple with just three control parameters and it would allow for higher operating frequencies. One

may further argue that solving the practical challenges in its control is much easier than building even a simple working quantum computer. It could, therefore, find use as a great test bench for the control techniques of superconducting qubits.

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Title

Control of Quantum Evolution and Josephson Junction Circuits

Abstract

Ever since Peter Shor's ground-breaking discovery in 1994 of an algorithm capable of factoring large integers on a quantum-mechanical computer exponentially faster than using any known classical method, research on quantum computing has boomed. Quantum information – a unique mixture of computer science, physics and mathematics – has developed into a new branch of information theory. On the experimental side, physicists from many different disciplines including atomic, solid-state and low-temperature physics, as well as optics, are striving today towards a practical quantum computer. All the candidate quantum bit (qubit) technologies have one thing in common: They rely on the controlled time-evolution of a closed quantum system, a seemingly paradoxical task.

In this Thesis the temporal control of quantum systems is studied. The topics included can be divided into two according to the type of temporal evolution; geometrical or dynamical. Geometrical realization-independent methods for quantum computing are studied first. Then the study is extended into dynamical quantum computing and the so-called Josephson charge-qubit register is considered as a test bench. Finally, a spin-off application of the geometrical evolution of a Josephson junction system is studied, i.e. Cooper pair pumping. A novel Cooper pair pump, the Cooper pair "sluice", is introduced.

The work on quantum computing reported in this Thesis is theoretical while the Cooper pair "sluice" is studied both theoretically and experimentally. Numerical simulations, both sequential and parallel, are used extensively throughout the Thesis. The experiments were carried out under cryogenic mK conditions and the sample fabrication was done using e-beam nanolithography.

Because the execution time of a quantum algorithm is always limited by the inevitable process of decoherence, it is important to utilize any measure available for accelerating quantum computations. It is found that practical quantum algorithms could greatly benefit from classical computer-aided optimization. Moreover, it is found that even a modest demonstrator of a full quantum algorithm using Josephson charge qubits is just barely realizable within present-day coherence times. However, the experimental part of this Thesis shows clear evidence of the functioning of the "sluice". While the worldwide effort of improving the coherence properties of qubits is underway, the "sluice" could well find practical use, e.g., in metrology in the foreseeable future.

Keywords
quantum systems, quantum mechanics, quantum computing, quantum algorithms, Cooper pair pumping

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