Entangling Qubits by Heisenberg Spin Exchange and Anyon Braiding

Daniel Zeuch
FLORIDA STATE UNIVERSITY
COLLEGE OF ARTS AND SCIENCES

ENTANGLING QUBITS BY HEISENBERG SPIN EXCHANGE AND ANYON BRAIDING

By

DANIEL ZEUCH

A Dissertation submitted to the
Department of Physics
in partial fulfillment of the
requirements for the degree of
Doctor of Philosophy

2016

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Daniel Zeuch defended this dissertation on May 31, 2016.
The members of the supervisory committee were:

Nicholas E. Bonesteel
Professor Directing Dissertation

Mark Sussman
University Representative

Vladimir Dobrosavljevic
Committee Member

Stephen Hill
Committee Member

Jorge Piekarewicz
Committee Member

The Graduate School has verified and approved the above-named committee members, and certifies that the dissertation has been approved in accordance with university requirements.
To my family.
ACKNOWLEDGMENTS

I owe my gratitude to all my friends who accompanied me while I lived in Tallahassee. Without them, today I would not be in the position to turn in a Ph.D. Dissertation and look forward to doing future work as a scientist.

During my life as a graduate student I have met many astonishingly delightful fellow students. I will never forget many pleasant evenings working on homework assignments at All Saints Café. Some of the physics students particularly close to me are Lakshmi Bhaskaran, Priyashree Roy, Raditya Utama, Sam Bein and, last but not least, Brendan and Tiara Diamond. I would also like to thank Radhika Vaidyanathan for often giving me a welcome distraction from the world of physics. I am also happy to thank my office mates and many others at the National High Magnetic Field Laboratory, such as the other students in our condensed matter study group and my fellow group members Julia Wildeboer, Robert Cipri, Weibo Feng and Luis Mendoza, for help with my work and for many stimulating dialogs that made my daily job more interesting. My friend and colleague Caitlin Carnahan is yet another person with whom it has been a pleasure work with. Finally, I believe that can call myself lucky that I have been supported by many of my friends from overseas, despite the change in time zone and the, oftentimes, unfortunate lack in regular contact. Among these are Angelika Steyer, Anna Stephan, Charlotte Schroer, Hannah Bos, Vanessa Knittel, Christoph Hanselka, Andreas Kaldun, and Martin Sommerfeld and many more.

The most crucial role in my evolution as a scientist has, beyond doubt, been played by my Ph.D. advisor Nick Bonesteel. Since the time when I first worked with him during a half-year long internship in 2009, he has always been excited to hear every detail of my findings (whenever there were any), and was constantly devoted to stressing the importance of critical thinking and logical rigor in presenting the work we have done. This, combined with his at times jovial attitude when discussing research, constituted a tremendous source of motivation for me. It further has to be said that my advisor never hesitated to respond to any of my questions or concerns regarding theoretical concepts by giving detailed explanations, and often proved to be quite patient when I was too stubborn to quickly follow his reasonings. For his numerous clarifications of physical concepts I am heavily indebted to him.
At this point I would also like to acknowledge my undergraduate thesis advisor at the University of Konstanz, Guido Burkard. I recall that the first time I got excited about the research field of quantum computation was in a class administered by him. It was also Guido Burkard who made my internship with Nick Bonesteel possible, and I have only positive memories of the time when I was working on my diploma thesis under his supervision.

For serving on my Ph.D. committee, I want to thank Mark Sussman, Stephen Hill, Vladimir Dobrosavljevic and Jorge Piekarewicz, and specials thanks to the latter two for their moral support over the last few years.

Finally, I want to express my deepest appreciation towards my entire family. They did not only let me go abroad without the slightest of complaints, but rather encouraged me to follow my dreams of studying and doing research, and they kept continuing their steady support for me, no matter what next steps I have considered to take. I am particularly happy because my father Klaus-Martin and my brother Valentin came to Tallahassee for a six-day visit when I defended my Dissertation.
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3.4 (a) Weave corresponding to phase seed $FR^4F$. (b) Weave obtained with this seed after one iteration of (3.10). (c) Weave obtained with this seed after a second iteration of (3.10). In (b) and (c) dashed lines divide parts of the weave corresponding to $U_k$ and $U_k^\dagger$ from those corresponding to the $R'$ and $R^3$ operations appearing explicitly in (3.10). For the seed $FR^4F$ the magnitude of the initial off-diagonal matrix elements is $x_0 \simeq 0.571$ and the initial phase is $\theta_0 \simeq 0.546\pi$. After two iterations $x_2 \simeq 8.30 \times 10^{-7}$ and $\theta_2 \simeq 0.488\pi$. (d) $\delta\theta$, shift in the phase of $\langle 0|U|0\rangle$ after one iteration of (3.10), plotted as a function of $x = |\langle 1|U|0\rangle|$, as well as $\Delta\theta^+$, $\Delta\theta^-$, and $\Delta\theta^\pm$ corresponding to different choices for the signs $s_k$ in (3.15). (e) Controlled-phase gate (see Fig. 3.3(b)) with $\theta_2 \simeq \theta_{\infty} \simeq 0.488\pi$ obtained using the second iteration phase weave shown in (c).

3.5 (a) Box representing an exchange weave, which in the $k \to \infty$ limit maps $|\star(\bullet\bullet)\rangle_1$ to $|\bullet(\star\bullet)\rangle_1$. (b) Controlled-$R^2$ gate construction for two three-anyon qubits.

3.6 (a) Weave corresponding to the exchange seed $FR^3F$. (b) Weave obtained with this seed after one iteration of (3.5). (c) Weave obtained with this seed after a second iteration of (3.5). For the seed $FR^3F$ the magnitude of the initial off-diagonal matrix elements is $x_0 \simeq 0.300$, and, after two iterations, $x_2 = 8.67 \times 10^{-14}$. In (b) and (c) dashed lines divide parts of the weave which corresponding to $U_k$ and $U_k^\dagger$ from those corresponding to the $R$ and $R^3$ operations appearing explicitly in (3.5). (d) Controlled-$R^2$ gate (see Fig. 3.5(b)) obtained using the second iteration exchange weave shown in (c). The controlled braid which enacts an $R^2$ operation only if the control qubit is the state 1 is indicated by the dashed box.
(a) Generalization of the class of two-qubit pulse sequences derived in Sec. 2.5 [shown in Fig. 2.22(a)] for which we have shown in that the Fong-Wandzura sequence is the optimal member.
ABSTRACT

As the discovery of quantum mechanics signified a revolution in the world of physics more than one century ago, the notion of a quantum computer in 1981 marked the beginning of a drastic change of our understanding of information and computability. In a quantum computer, information is stored using quantum bits, or qubits, which are described by a quantum-mechanical superposition of the quantum states 0 and 1. Computation then proceeds by acting with unitary operations on these qubits. These operations are referred to as quantum logic gates, in analogy to classical computation where bits are acted on by classical logic gates. In order to perform universal quantum computation it is, in principle, sufficient to carry out single-qubit gates and two-qubit gates, where the former act on individual qubits and the latter, acting on two qubits, are used to entangle qubits with each other.

The present thesis is divided into two main parts. In the first, we are concerned with spin-based quantum computation. In a spin-based quantum computer, qubits are encoded into the Hilbert space spanned by spin-$\frac{1}{2}$ particles, such as electron spins trapped in semiconductor quantum dots. For a suitable qubit encoding, turning on-and-off, or “pulsing,” the isotropic Heisenberg exchange Hamiltonian $J \mathbf{S}_i \cdot \mathbf{S}_j$ allows for universal quantum computation and it is this scheme, known as exchange-only quantum computation, which we focus on. In the second part of this thesis, we consider a topological quantum computer in which qubits are encoded using so-called Fibonacci anyons, exotic quasiparticle excitations that obey non-Abelian statistics, and which may emerge in certain two-dimensional topological systems such as fractional quantum-Hall states. Quantum gates can then be carried out by moving these particles around one another, a process that can be viewed as braiding their 2+1 dimensional worldlines.

The subject of the present thesis is the development and theoretical understanding of procedures used for entangling qubits. We begin by presenting analytical constructions of pulse sequences which can be used to carry out two-qubit gates that are locally equivalent to a controlled-PHASE gate. The corresponding phase can be arbitrarily chosen, and for one particular choice this gate is equivalent to controlled-NOT. While the constructions of these sequences are relatively lengthy and cumbersome, we further provide a straightforward and intuitive derivation of the shortest known two-qubit pulse sequence for carrying out a controlled-NOT gate. This derivation is carried out
completely analytically through a novel “elevation” of a simple three-spin pulse sequence to a more complicated five-spin pulse sequence.

In the case of topological quantum computation with Fibonacci anyons, we present a new method for constructing entangling two-qubit braids. Our construction is based on an iterative procedure, established by Reichardt, which can be used to systematically generate braids whose corresponding operations quickly converge towards an operation that has a diagonal matrix representation in a particular natural basis. After describing this iteration procedure we show how the resulting braids can be used in two explicit constructions for two-qubit braids. Compared to two-qubit braids that can be found using other methods, the braids generated here are among the most efficient and can be obtained straightforwardly without computational overhead.
CHAPTER 1
INTRODUCTION

The purpose of this introductory chapter is twofold: first, to provide some historical context as well as my own personal perspective on the relatively new field of quantum computation; and second, to present some necessary background material for the reader to understand the results given in Chapters 2 and 3.

1.1 Historical Remarks

“And I’m not happy with all the analyses that go with just the classical theory, because nature isn’t classical, dammit, and if you want to make a simulation of nature, you’d better make it quantum mechanical, and by golly it’s a wonderful problem, because it doesn’t look so easy.”

—Richard Feynman, 1981

The emergence of quantum mechanics in the early twentieth century deeply enhanced our understanding of many physical phenomena. Despite the fact that the world around us can be widely explained and predicted by the theory of quantum physics, it took over a half century before it was proposed that the same theory could be exploited to widen the horizon of what we consider “efficiently computable.”

In 1981, Richard Feynman introduced the notion of a quantum computer [1], a new kind of machine whose computational process would be described quantum mechanically rather than classically. He suggested that such a computer could be used to efficiently simulate certain quantum systems that cannot be simulated with an ordinary, or classical, computer.

Progress in the theory of quantum computers was initially slow, with only a small group of researchers following Feynman’s remarkable suggestion. Indeed, it took several years until the first precise model of a quantum computer was described by David Deutsch [2, 3]. It was still later, in the mid-1990s, that a number of quantum algorithms were discovered which showed that quantum computers could solve certain problems that no classical computer could solve.
This discovery of the potential power of quantum computers led to an explosion of interest, both theoretical and experimental, which has continued unabated to this day. It was immediately apparent that, given the delicate nature of quantum states, it would be necessary to provide quantum computers with some kind of robustness against errors and the loss of quantum coherence. This led to the development of so-called quantum error correction.

We now give a sketch of some of the historical milestones that have led to the current knowledge and views of the field of quantum computation and quantum information.\(^1\)

### 1.1.1 Before the 1990s

The number of particles contained in a macroscopic system is typically on the order of Avogadro’s number. To analytically determine the physical behavior of such a complex system (i.e., make predictions about quantities like density, conductivity, heat capacity or magnetization), keeping track of the degrees of freedom of every particle is intractable even for purely classical calculations. It therefore proves indispensable to use extensive approximations before being able to solve such kind of problems. It is often not a simple process to determine which kind of approximations, on the one hand, allow one to solve a given problem and, on the other hand, do not obscure fundamental characteristics of the system in question.

When known analytical methods fail to describe experimental findings, a popular alternate route to acquire insight into how physical phenomena emerge is to simulate physical systems on a computer. In this context, a natural question arises: which physical systems can be numerically simulated? Feynman addressed this question in his “keynote speech” in 1981 [1] at the First Conference on Physics and Computation, held at MIT. As Feynman discussed, suppose we are able to numerically simulate the time evolution of a given physical system of particles using a given amount of resources such as computation time, hard disc space and so on. We can then ask the following question: if we increase the size of the system, then does the amount of resources required to simulate the larger system grow only polynomially in the amount of increase, or is this growth exponential? If the growth in required resources for a given system is exponential, clearly, we do not have the ability to simulate large systems efficiently.

\(^1\)In writing this historical sketch I have been influenced by a talk given by Feynman [1] and by a book written by Scott Aaronson [4].
It seems natural to think that the answer to this question depends on the type of computer used to carry out the simulation. It turns out, however, that all classical computing devices (such as different kinds of desktop computers, notebooks or cell phones) are, in this respect, equivalent to each other and so the answer to the above question is independent of the computer used for the simulation. The discovery that all classical computers are equivalent goes back to the 1930s when Church and his student, Turing, made an important contribution to the theory of computer science by showing the equivalence of various definitions of computability.\(^2\)

One of the definitions of computability, put forward by Alan Turing in 1936, is based on an abstract computing device known as the Turing machine,\(^3\) which describes a very simple computer whose working principle we now summarize. This machine consists of a segmented tape and a control unit which can move, segment by segment, along the tape. Each segment of the tape is occupied by a number, such as 0 or 1, and so the tape can be understood as a digital memory. During the computing process the control unit, which has a given set of instructions, reads out the values of the segments on the tape, and may change these values depending on the control unit’s state of computation. When the machine has finished its calculation, it will write its result to some designated area of the tape, and after that it will halt.

A “universal” Turing machine\(^4\) is a particular kind of Turing machine that can be used to simulate any other computing device, and it is often used as the standard object of comparison when considering the complexity of computer algorithms. Of course, the fact that a Turing machine is universal does not, by any means, imply that it can solve any arbitrary problem. Along with proposing the Turing machine and pointing out its usefulness for characterizing the concept of computability, Turing himself elegantly proved that the Turing machine cannot solve the “halting problem.” This problem is to answer the question if a given computer program halts after a finite amount of time (or otherwise it may be trapped in an infinite calculation loop). As we will see below, the notion of universality is also central in the discussion to the theory of quantum computation.

The Church-Turing thesis states that any function that is naturally regarded as being “computable” can be computed by a Turing machine. Note that the Church-Turing thesis may be regarded as an empirical statement about reality. As a practical matter, however, we should go

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\(^3\)https://en.wikipedia.org/wiki/Turing\_machine

\(^4\)https://en.wikipedia.org/wiki/Universal\_Turing\_machine
beyond the question of “computability per se” by asking which functions are efficiently computable. Following Feynman, we say that a function can be calculated efficiently if the time it takes to do so does not increase exponentially in the input of that function. The extended, or physical, Church-Turing thesis then states that any function that is efficiently computable can be computed by a Turing machine [2].

The extended Church-Turing thesis, like the Church-Turing thesis itself, can be viewed as an empirical claim that may, in principle, be falsified. Is there a good reason to think that Turing machines cannot efficiently simulate nature? Indeed, a system that, on a first glance, surely seems difficult to simulate is one that behaves quantum-mechanically. An argument for why this is the case is that the Hilbert space of quantum mechanical particles, such as spin-1/2 particles, grows exponentially in the number of particles. But the storage space available to a Turing machine is only linear in the length of the “memory” strip. Clearly, the requirement of an exponentially large memory rules out the possibility to store all quantum mechanical amplitudes of a many-particle system on a computer.

This is a good point to return to Feynman’s talk [1], in which he considered the possibility of simulating quantum-mechanical systems using probabilistic computers which work using some probability distribution rather than quantum mechanical amplitudes. He then refers to the Einstein-Podolsky-Rosen paradox, which inspired the discovery of Bell-type inequalities in the 1960s which draw a clear discrepancy between classical and quantum-mechanical predictions for certain measurable quantities [5]. Subsequent related experiments confirmed that quantum theory is inherently different from classical “hidden-variable” theories, that is, theories that are based on the notion that the state vectors that describe particles are always completely determined although some of these variables may sometimes be hidden from the observer. Based on this discrepancy between classical and quantum computation, Feynman concludes that there are quantum mechanical systems that cannot be imitated accurately by classical computers.

In the same talk [1], Feynman further devotes what he calls a “side-remark” to point out why he believes that using a quantum mechanical two-level system — known today as a “qubit” — in a computing device can be used to simulate other quantum systems. He points out that his “quantum simulator” is “not a Turing machine, but a machine of a different kind.”
A quantum computer similar to that of Feynman has then been introduced by Deutsch in 1985 [2]. In the spirit of Feynman’s approach, he showed that the quantum computers that he describes are able to simulate arbitrary quantum systems. In Deutsch’s view, his own “true ‘computer’” will calculate any arbitrary function including any desired dynamical laws while Feynman’s computer evolves under certain predefined and constant physical laws. Because of this, Deutsch’s quantum computer is able to simulate arbitrary quantum systems, or in other words, it is like a universal quantum Turing-machine.

In 1989, Deutsch then presented a generalization of the circuit model of classical computers in which every entry in the memory of the computer is in a quantum superposition [3]. While the fundamental unit of information in classical memory is the bit, which can be either in the state 0 or 1, its generalization, the quantum bit, or short “qubit” after Schumacher [6], is then described by a superposition of quantum states $|0\rangle$ and $|1\rangle$. Data is then processed by enacting circuits of “quantum gates” on the system of qubits. As explained in Secs. 1.2.1 and 1.2.2, quantum computation may in principle be carried out by using only so-called single-qubit gates and two-qubit gates where, as these names imply, a single-qubit gates act on one qubit at a time and two-qubit gates act on pairs of qubits.

1.1.2 The 1990s

There are two main reasons for why the mere notion of a universal quantum computer did not very quickly spark a huge amount of excitement. First, it was not clear what a quantum computer might be particularly useful for, other than simulating quantum systems as had been suggested by Feynman [1]. Second, while in the early 1990s there was no clear picture of how such a device would in practice actually look like, it quickly became apparent that even if one had such a quantum computer then carrying out calculations would only be feasible if there is some way to protect the computer’s stored information from interactions with the environment and resulting errors.

In 1985, Deutsch had already described a quantum algorithm [2] that solves the following problem: consider a function $f$ that maps the set $\{0, 1\}$ to the very same set, $\{0, 1\}$. The possible functions can be divided into two groups, where group (i) contains the functions $g$ which map 0 and 1 to different values [i.e., $g(0) \neq g(1)$] and group (ii) contains the functions $h$ which map 0 and 1 to the same value [i.e., $h(0) = h(1)$]. To solve the problem of finding out if a given function $f$ belongs to group (i) or (ii), a classical computer clearly needs to query the function $f$ twice to calculate both
values \( f(0) \) and \( f(1) \) and then compare them. Deutsch presented a quantum algorithm that makes use of quantum entanglement and interference in order to solve this problem with only a single query of \( f \) [2]. A quantum algorithm, discovered in 1992, that can be used to solve a generalized problem is known as the Deutsch-Josza algorithm [7].

In 1994, Shor found a prime-factoring algorithm which, if executed on a quantum computer, achieves an exponential increase in computing speed over the best known classical factoring algorithms [8]. Due to its applicability to decode a commonly used encryption method for data transfer, known as RSA encryption, Shor’s algorithm began to draw interest from the general public to the topic of quantum computation. In 1997, Grover found a quantum algorithm which allows for searching a database with \( N \) entries for a single entry within \( \sqrt{N} \) computation steps [9]. Grover’s algorithm thus provides a quadratic increase in computing speed compared to the best possible classical algorithm, which necessarily requires on the order of \( N \) steps.\(^5\) There have been discoveries of many other quantum algorithms, and a comprehensive overview over the known algorithms can be found at the zoo of quantum algorithms composed by Stephen Jordan.\(^6\)

Only a year after Shor’s celebrated display of the capability of quantum computing, the first significant steps towards stabilizing quantum information were made. In the mid 1990s, it was realized that storing information in many degrees of freedom allows one to detect and correct errors without altering the stored quantum information. The first two quantum error correcting codes which can be used to store and manipulate quantum computation fault-tolerantly were published in 1996 by Shor\(^7\) [10] and Steane [11].

An important cornerstone in the history of quantum error correction was marked by the threshold theorem which was formulated independently by a number of authors [12, 13, 14, 15]. This theorem states that ideal quantum computations can be approximated to arbitrary precision using faulty computer components, such as quantum gates, provided the error rate for each of these gates,

\(^5\)Grover’s algorithm is not a prerequisite for understanding the results described in the main part of this thesis (Chapters 2 and 3). Nonetheless, in Sec. 1.2.3 we discuss how Grover’s algorithm proceeds because this exercise gives a flavor of how a quantum computer exploits the exponential degrees of freedom associated with the Hilbert space of qubits.

\(^6\)http://math.nist.gov/quantum/zoo/

\(^7\)Based on an error correction code related to the Shor code [10], Sec. 1.2.4 explains how one may in principle determine and correct errors without loss of information. We note that knowing the details of quantum error correction is (as Grover’s algorithm) not vital for understanding the main part of this thesis. We still decided to include this explanation because this topic is crucial for any experimental realization of a large-scale quantum computer.
\( \epsilon \), is below a certain threshold \( \epsilon_0 \). In 1997, this threshold was estimated to be at most \( \epsilon_0 \sim 10^{-6} \) [12], which would imply that satisfactory quantum gates need to operated with a success rate of of at least \( 1 - \epsilon_0 \approx 99.999\% \). However, different underlying quantum error correcting codes yield different thresholds, and over the following years the quality requirements on quantum gates became less stringent.

Yet still, at the end of the 20th century many regarded the problem of decoherence as a major obstacle, and it was studied in greater detail by, for example, Landauer [16] and Unruh [17]. It was cautioned against being too hopeful that the problem of decoherence could one day seriously be overcome. A short article from the same time that makes for pleasant bedtime reading is titled “Quantum Computing: Dream or Nightmare?” by Haroche and Raimond [18]. These authors argue that since quantum error correction schemes require a significant overhead in additional resources and computation steps, the exponential increase in computing power will become noticeable only for a very large number of qubits. Hence, if one, for example, wants to factor a number that is on the order of \( 10^{10} \), then to do this it might very well be less costly to build a significantly better classical computer rather than a quantum computer.

1.1.3 The New Millennium

Despite the criticism of quantum computation expressed in the 1990s, the discovery that quantum errors might be successfully dealt with urged more researchers to pursue the quest of actually building and operating small-scale prototype quantum computers in the laboratory. Since a qubit can be represented by any quantum two-level system, the list of potential qubits is long. Among the more prominent proposals [19] are those in which qubits are represented by photons, trapped ions, nuclear spins manipulated by NMR or integrated circuits, better known as superconducting qubits. Furthermore, there are two other promising approaches, both of which are central to the main part of this thesis. In one, a qubit is represented by one or more spin-1/2 particles, such as the spins of electrons captured in semiconductor quantum dots. In the other approach, a qubit is represented by rather exotic particles that obey non-Abelian statistics. We now state some key ideas of each of these proposals.

Photons can be used as qubits by, for example, encoding the qubit states 0 and 1 into the photon polarizations as shown in Fig. 1.1(a). The qubit states of a photon can thus be manipulated using waveplates, enabling single-qubit gates. Allowing photons to interact in order to realize two-qubit
Figure 1.1: Basic information for various qubits. In (a), the horizontally and vertically polarized photons denote the qubit states $|0\rangle$ and $|1\rangle$, respectively, and a circular polarized photon is in the state $|0\rangle + i|1\rangle$. Part (b) shows the molecule of alanine, which has been used in demonstrations of NMR quantum computation in which the Deutsch-Jozsa algorithm [7] was carried out with three qubits [22, 23]. Each qubit is represented by one of the three black carbon atoms (Source: Wikipedia, 2016 [24]). Part (c) shows a schematic view of an ion trap (Source: Institut für theoretische Physik, Universität Innsbruck, 2016 [25]). Finally, part (d) shows an example of a superconducting qubit consisting of a circuit in which a capacitor and a Josephson junction (denoted by the “X”) are connected, together with the corresponding anharmonic potential for which the energies of the ground and first excited states correspond to the qubit states. This particular qubit has been named the Cooper-Pair box [26].

Gates is more complicated. Nonetheless, in 2001, Ref. [20] showed how arbitrary quantum gates can theoretically be carried out using merely linear optical circuits. On the experimental side, in 2009 a first demonstration of Shor’s algorithm on a photonic chip has been reported in Ref. [21].

The long history of research and applications of nuclear magnetic resonance (NMR) techniques has been combined with the theory of quantum information [27, 28]. Here, molecules dissolved in liquids are used to host qubits — the different nuclear spins of the atoms of the molecule — and quantum gates are carried out via NMR pulses. As an example, Fig. 1.1(b) shows a molecule that has been used in certain experiments of NMR based quantum computation [22, 23, 24]. Conceptually, the most substantial problem that had to be overcome was that the quantum state of the macroscopic number of molecules dissolved in a test tube is described by a density matrix and, naively, a measurement of such an ensemble state does not seem very useful compared
to the measurement of a single qubit occupying a pure state [27, 28, 29]. Still, in as early as 2001, NMR-based quantum computation has been used to factor the number 15 [30]. However, the capabilities of this scheme are limited mainly because of the difficulty to synthesize arbitrarily large molecules while at the same time addressing individual spins with NMR pulses.

One of the earliest experimental realizations of a few-qubit system is based on the idea of representing qubits by ions or atoms confined in harmonic traps (such as Penning or Paul traps for ions, and purely magnetic traps for atoms). Qubit states can be encoded into the spin- and motion-degrees of freedom of the ions (or atoms), and quantum gates can be mediated via a combination of laser pulses and collective motion [31]. A schematic picture of a trap hosting a number of ions that are manipulated by a laser beam is shown in Fig. 1.1(c) [25]. In 1995, after this topic had just been theoretically introduced [32], an experimental realization of an entangling two-qubit gate was reported [33]. Experimental progress in this area is exemplified by an experiment in 2005 where a total of eight Calcium ions were confined to a linear array [34], and further by a more recent experimental demonstration of a two-dimensional array of 49 Caesium atoms used as qubits [35].

Part of the difficulty in manipulating qubits is given by the microscopic spatial dimensions of the quantum two-level system at hand. An exception to the rule is the superconducting qubit, which was first propagated in 1997 [36, 37, 38]. To understand how an electric circuit can be used as a quantum two-level system, consider a simple \( LC \) circuit. If all components in this circuit are built of superconductors, the current flow is free of dissipation so the usual approximation of zero resistance actually becomes exact, and the system is correctly described by a harmonic oscillator. The energy levels of this circuit are then given by \( \hbar \omega (n + 1/2) \) (with the Planck constant \( \hbar \), integers \( n \) and the resonance frequency \( \omega = 1/\sqrt{LC} \) where \( L \) and \( C \) is the inductance of the inductor and the capacitance of the capacitor). If the energy levels were not equidistant one could use the, say, lowest two energy levels as a qubit. Now assume we extend the \( LC \) circuit by adding a Josephson junction — an electronic component that consists of two weakly coupled superconducting regions. This junction introduces desired anharmonicities into the spectrum, opening the possibility to use the circuit as a qubit. As an example, Fig. 1.1(d) shows a minimal electric circuit for a superconducting qubit in which a capacitor and a Josephson junction are connected, together with the circuit’s anharmonic potential. Manipulations of these states depend strongly on the type of the qubit. Many variations of integrated circuits were reported since the end of the 20th century.
(for example, see Refs. [26, 39, 40]), and to this day superconducting qubits are subject to active ongoing research.

In 1998, Loss and DiVincenzo put forward a quantum computation proposal [41] that counts among the most promising still today. They envisioned to let a qubit be represented by the spin of an electron that is isolated in some region within a semiconductor heterostructure. A convenient choice to represent the qubit states 0 and 1 are the up and down states of each electron spin, and this spin-degree of freedom can then be manipulated by applying local magnetic fields. Two-qubit gates can be carried out by letting the electron wave functions overlap and thereby turning on the Heisenberg exchange Hamiltonian $\mathcal{H} = J \mathbf{S}_1 \cdot \mathbf{S}_2$ acting two spin-$1/2$ particles, where $J$ is the exchange coupling strength. Given the electric charge of an electron, the overlap of two electrons can be readily controlled by applying electric fields and the first experiment in which this Hamiltonian has been coherently turned on-and-off, or “pulsed,” has been reported in 2005 by Petta et al. [42]. [An explanation of how this exchange Hamiltonian may be pulsed is given in Sec. 1.3.1.] As was already noted in Ref. [41], addressing individual spins to carry out single-qubit rotations is a much more difficult task than pulsing the exchange Hamiltonian. Nonetheless, after the initial realization of a two-qubit gate by Petta et al. [42], experiments were reported in which single-qubit gates as well as two-qubit gates were demonstrated [43, 44, 45]. Still, single-qubit gates carried out this way are slower than two-qubit gates and will require more experimental overhead [46].

Shortly after the original Loss-DiVincenzo spin-based quantum computer, two similar theoretical proposals were published in 2000 [47, 48] and 2002 [49]. In the earlier of these two, quantum gates are carried out solely by pulsing the exchange Hamiltonian between pairs of spins. For these constraints, DiVincenzo et al. [46] provided the first explicit computation scheme in which each logical qubit is encoded using three spins. In the other proposal [49], Levy suggested to encode logical qubits using pairs of spins and to carry out arbitrary quantum gates by using exchange pulses combined with gradients in Zeeman fields. Both of these proposals of Refs. [47, 48] and 2002 [49] achieve a decrease in experimental overhead for carrying out quantum gates while increasing the number of spins that represent the logical qubits. In Chapter 2 we focus on the computation scheme of Refs. [46, 47, 48].

The last quantum computing proposal that we describe can be regarded as more speculative than the proposals mentioned above. This is because the particles proposed to represent logical
qubits have not yet been directly experimentally observed. Such particles obey non-Abelian statistics and may appear in two-dimensional topologically ordered systems, for example as quasiparticle excitations known as non-Abelian anyons in certain fractional quantum Hall states [50, 51]. Associated with these non-Abelian particles there is a Hilbert space whose dimension is exponentially large in the total number of particles present. These particles can therefore be used to represent qubits. Further, information is stored non-locally within this Hilbert space, providing the system of anyons with an inherent “topological protection” from local perturbations.

The non-Abelian particles can then be moved around one another, a process known as braiding the 2+1 dimensional worldlines of the particles, which results in transitions from one state within the Hilbert space to another. Because of this, a system of non-Abelian particles is a suitable platform for so-called topological universal quantum computation [52, 53, 51]. [In Sec. 1.3.2 we provide a graphic description of the concept of braiding and the associated topological protection within the Hilbert space of non-Abelian particles.] An article published in Scientific American that vividly introduces this vast and interesting topic is titled “Computing with Quantum Knots” [54].

Different quasiparticle types have different properties. For example, the most well-known non-Abelian quasiparticles whose experimental realization is currently being actively pursued (see, for example, the review in Ref. [55]) are so-called Majorana zero modes. However, the set of unitary operators produced by braiding these particles is insufficient for universal quantum computation. The so-called Fibonacci anyon, however, is a type of non-Abelian particle for which, in the year 2002, braiding has been shown to be universal [53]. Three years prior to this finding, Read and Rezayi discovered a wave function that may describe certain fractional quantum Hall states, and this wave function admits quasiparticle excitations that are Fibonacci anyons [56, 57]. While there has not been concrete experimental evidence on finding these kind of particles, there were theoretical studies on how to carry out single- and two-qubit gates. The first explicit work on how to efficiently find braid patterns that result in desired gate operations was published in 2005 by Bonesteel et al. [58].

One measure for the quality of qubits is the coherence time, which is a measure for how much time passes before quantum information stored in a qubit becomes inaccessible due to unwanted couplings with the environment. Figure 1.2 shows a plot of the best so-called $T_2$ coherence times of superconducting qubits reported between 1999 and 2011. This graph shows that within the first
Figure 1.2: Plot of the best $T_2$ coherence times measured between 1999 and 2011 for superconducting qubits [59]. The reproducible coherence times, indicated by dark blue dots, follow a trend of a remarkable exponential increase (dashed line) over the years between 2005 and 2011.

In Sec. 1.1.2 we pointed out that an important primitive for quantum computation are so-called quantum error correcting codes. One of the most promising error correcting codes has been introduced in 1998 by Bravyi and Kitaev and is known as the surface code [60]. As the name implies, it is based on a two-dimensional square lattice, a “surface,” of physical qubits for which nearest-neighbor gates can be implemented. This code constituted a considerable step forward toward a long-lasting quantum memory. In 2007, Raussendorf and Harrington extended the surface code by describing how a certain set of single-qubit and two-qubit operations — known as the Clifford group — can be carried out fault-tolerantly [61, 62]. Even though the Clifford group is by itself not sufficient for universal quantum computation, this error correction scheme allows for error thresholds that are on the order of $\epsilon_0 \sim 1\%$, and it is one of the most prominent codes known to this
Figure 1.3: Bloch sphere, providing a mapping from the two-dimensional Hilbert space of a qubit to a spin-1/2 pseudospin. In this mapping, the $|0\rangle$ and $|1\rangle$ states [shown in (a)] are mapped to the $+\hat{z}$ and $-\hat{z}$ unit vectors [compare with (b)], respectively. Similar, the $\pm \hat{x}$ vectors correspond to $(|0\rangle \pm |1\rangle)/\sqrt{2}$, and the $\pm \hat{y}$ vectors [not shown in (a)] are mapped to $(|0\rangle + i|1\rangle)/\sqrt{2}$.

A useful generalization of the surface codes that we just mentioned was worked out by Koenig et al. [64] in the year of 2010. These generalized codes, also referred to as non-Abelian surface codes, are related to certain spin lattice models which exhibit a topological phase that supports Fibonacci anyons [65]. Similarly, Fibonacci anyons may be created in the quantum error correcting codes identified by Koenig et al., and it turns out that moving these anyons around one another can be done fault-tolerantly. Since, as discussed above, braiding Fibonacci anyons results in a set of quantum gates that is universal, the non-Abelian surface codes can be used for fault-tolerant universal quantum computation by anyons.

This concludes our account of the history of quantum computation. In Sec. 1.2 we explain some of the fundamental theoretical notions of quantum computation. Finally, in Sec. 1.3 we describe how quantum gates are carried out in the two computing schemes discussed in the main part of this thesis.
1.2 How Does a Quantum Computer Work

The general theory of quantum computation is discussed in the book of Ref. [66]. Here we discuss some of the most fundamental theoretical concepts necessary for understanding the importance of the methods developed in this thesis. In Secs. 1.2.1 and 1.2.2 we first explain the qubit Hilbert space and the most fundamental quantum gates, and describe the quantum circuit model. Section 1.2.3 then gives a tutorial on Grover’s search algorithm [9] as an example of how the exponentially many degrees of freedom associated with some number of qubits may be exploited to gain a significant increase in computational power using a quantum computer. In Sec. 1.2.4, we show how qubit errors may in principle be detected and corrected.

1.2.1 Single-Qubit Rotations

Figure 1.3 illustrates the Bloch sphere. In Fig. 1.3(a) the two-dimensional qubit Hilbert space, spanned by the orthogonal states $|0\rangle$ and $|1\rangle$, is mapped onto the geometrical unit sphere shown in (b). The fact that qubit state vectors reside within the unit sphere is reflected in the normalization condition $|\alpha|^2 + |\beta|^2 \leq 1$. The mapping of a state $|\psi\rangle$ of unit magnitude in pseudospin coordinates in terms of the polar angle $\theta$ and the azimuthal angle $\phi$, as shown in Fig. 1.3(a), is given by

$$ |\psi\rangle = \cos(\theta/2)|0\rangle + \sin(\theta/2)e^{i\phi}|1\rangle = \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2)e^{i\phi} \end{pmatrix}, \quad (1.1) $$

where for the second equality sign we identify $|0\rangle = (1,0)^T$ and $|1\rangle = (0,1)^T$. To ensure consistency with Fig. 1.3, here in this mapping the overall phase is chosen such that for an arbitrary state $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ the coefficient $\alpha$ is real. In the following, qubit states may be multiplied by overall phase factors which are, however, meaningless whenever the qubit is not in an entangled state.

Unitary operations acting on a single qubit are often called single-qubit rotations because they can be viewed as rotations of the qubit state vector around the Bloch sphere. The operators corresponding to single-qubit rotations can be classified as group elements of the unitary group of operators $U(2)$. Consider a unitary operator acting on a qubit in state $|a\rangle$. We can identify this as a Bloch sphere rotation about an axis $\hat{n} = (n_x, n_y, n_z)$ whose matrix representation in the basis
$a = \{0, 1\}$ is given by

$$e^{-ia/2} \exp \left( i \frac{\alpha}{2} \hat{n} \cdot \sigma \right) = e^{-ia/2} \text{1}_2 \cos \left( \frac{\alpha}{2} \right) + i e^{-ia/2} \hat{n} \cdot \sigma \sin \left( \frac{\alpha}{2} \right)$$

$$= e^{-ia/2} \left( \cos \left( \frac{\alpha}{2} \right) + in_z \sin \left( \frac{\alpha}{2} \right) \begin{array}{cc}
in_x - ny \\ \cos \left( \frac{\alpha}{2} \right) - in_z \sin \left( \frac{\alpha}{2} \right) \end{array} \right). \quad (1.2)$$

In the above equation (1.2), $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ $\text{1}_2$ is the Pauli spin vector and $\text{1}_2$ is the $2 \times 2$ identity operation. In the following, all matrix representations of single-qubit gates are given in this standard qubit basis $\{ |0\rangle, |1\rangle \}$.

There is only one nontrivial classical single-bit operation: the bit flip gate, or NOT gate, which maps the classical states 0 and 1 to 1 and 0, respectively. In the quantum regime, we denote this gate by $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, again given in the standard basis $\{ |0\rangle, |1\rangle \}$. This NOT gate then carries out a $\pi$ rotation about the $x$ axis, as can be seen from Eq. (1.2) for $\hat{n} = \hat{x}$ and $\alpha = \pi$, and its action on a qubit is given by

$$X(\alpha |0\rangle + \beta |1\rangle) = (\beta |0\rangle + \alpha |1\rangle). \quad (1.3)$$

Two other fundamental gates are the phase flip gate, $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, and the gate which corresponds to a phase flip followed by a bit flip, $Y = XZ = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$. The action of a phase flip gate is a $\pi$ rotation about the $z$ axis, and can be written as

$$Z(\alpha |0\rangle + \beta |1\rangle) = (\alpha |0\rangle - \beta |1\rangle). \quad (1.4)$$

Similarly, the action of the operator $Y$ is a $\pi$ rotation about the $y$ axis. In Sec. 1.2.4 we will discuss the basic notion of detecting and correcting single-qubit errors which may be divided into discrete errors described by the operators $X$, $Y$ and $Z$. We will see how one type of errors may be corrected by a relatively simple procedure.

Figure 1.4(a) illustrates how single-qubit gates are represented in the quantum circuit model. Shown are a generic gate as well as the bit flip gate $X$, together with yet another noteworthy single-qubit gate, known as the Hadamard gate, $H$. Its action on a qubit is a $\pi$ rotation about the axis along $\hat{x} + \hat{z}$. The matrix representation in the standard qubit basis is given by $H = \frac{1}{\sqrt{2}}(X + Z) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$. The corresponding action, as shown in Fig. 1.4(a), on a state $|0\rangle$ is to map it to an equal superposition of the states $|0\rangle$ and $|1\rangle$ with zero phase difference. This gate will below be useful in the discussion of two-qubit gates and quantum algorithms.
1.2.2 Two-Qubit Gates

Two-qubit gates are used to entangle pairs of qubits with each other. An entangled state of two qubits is defined as a state that cannot be written as a product state of the qubits, such as \( |00\rangle \equiv |0\rangle \otimes |0\rangle \) or \(|01\rangle + |00\rangle \equiv |0\rangle \otimes |0\rangle + |0\rangle \otimes |1\rangle = |0\rangle \otimes (|1\rangle + |0\rangle)\). For an example of an entangled state, consider the two-qubit state \(|00\rangle + |11\rangle\) which, clearly, cannot be factorized into a state of the form \(|\psi_1\rangle \otimes |\psi_2\rangle\) where \(|\psi_1\rangle\) and \(|\psi_2\rangle\) are quantum states describing two different qubits. The operators corresponding to these kind of gates belong to the group U(4), and one particular type of these gates are known as controlled-operation gates. Figure 1.4(b) shows a circuit diagram of such a controlled-\(U\) gate acting on a control qubit, labeled 1 in the figure, and a target qubit, labeled 2. The matrix representation of such a gate acting on a control qubit in state \(|a\rangle\) and a target qubit in state \(|b\rangle\) can be given in the basis \(a = \{0, 1\}\) as

\[
U_{\text{2qubit}} = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & U \end{pmatrix}
\]

(1.5)

where the \(2 \times 2\) matrices \(\mathbb{1}_2\) and \(U\) act on the Hilbert space of the target.

A canonical two-qubit gate is the \textsc{cnot} gate whose circuit representation is given in Fig. 1.4(b). If we enact this gate on a control qubit with state label \(a\) and target qubit with label \(b\), its action
Figure 1.5: Local equivalence between CNOT and controlled-Z gates. As explained in the text, a controlled-Z gate preceded and followed by Hadamard gates acting on the (lower) target qubit has the same effect as CNOT.

depends on the control qubit and can be given as

$$|a = 0 \rangle |b \rangle \xrightarrow{\text{CNOT}} |a = 0 \rangle |b \rangle, \quad |a = 1 \rangle |b \rangle \xrightarrow{\text{CNOT}} |a = 1 \rangle |b + 1 \rangle.$$  (1.6)

This action can be summarized by writing $$|a \rangle |b \rangle \xrightarrow{\text{CNOT}} |a \rangle |b \oplus a \rangle$$, where $$\oplus$$ denotes addition modulo 2, as also given in Fig. 1.4(b). In other words, the action of CNOT on the target is either the identity if $$a = 0$$, or a NOT operation if $$a = 1$$. The corresponding matrix representation in the two-qubit basis with state ordering $$ab = \{00, 01, 10, 11\}$$ is then

$$U_{\text{CNOT}} = \begin{pmatrix} 1 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 \end{pmatrix}.$$  (1.7)

To understand how CNOT can be used to entangle a pair of qubits, acted on a control qubit in state $$|0 \rangle + |1 \rangle$$ and a target qubit in state $$|0 \rangle$$. According to Eq. (1.6) we find that the action of a CNOT gate onto these initially unentangled qubit states is to entangle them,

$$\left(|0 \rangle + |1 \rangle\right) \oplus |0 \rangle = |00 \rangle + |10 \rangle \xrightarrow{\text{CNOT}} |00 \rangle + |11 \rangle.$$  (1.8)

It is for this reason that CNOT is called an entangling two-qubit gate.

It has been shown that being able to (i) arbitrarily rotate single-qubit states around the Bloch sphere and (ii) entangle qubits using a CNOT gate allows for universal quantum computation [67]. This gate set consisting of arbitrary single-qubit rotations and CNOT is, however, not particularly practical because it is inconceivable how to carry out an infinite number of single-qubit rotations to arbitrary precision. A more pragmatic set of gates is a finite subset of this universal set, such as the set consisting of Hadamard $$H$$, a $$z$$-axis rotation through angle $$\pi/8$$ [see Eq. (1.2) for $$\hat{n} = \hat{z}$$] and CNOT [66].
It is important to note that different two-qubit gates may be related to each other by single-qubit rotations. For example, consider the two-qubit controlled-$Z$ gate acting on two qubits in states $|a\rangle$ and $|b\rangle$, with matrix representation in the standard two-qubit basis $ab = \{00, 01, 10, 11\}$,

$$U_{\text{controlled-}Z} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ -1 \end{pmatrix}.$$  \hfill (1.9)

This gate acts as the identity and as a $Z$ operation if $a = 0$ or $1$, respectively. As shown in Fig. 1.5, one obtains a CNOT gate by carrying out a Hadamard gate on the target qubit before and after the controlled-$Z$ operation. To show this, note that if the control qubit is in state $a = 1$, the sequence of operations is given by

$$H Z H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$  \hfill (1.10)

To carry out the same calculation for the case where the control qubit is in state $a = 0$, first note that the controlled-$Z$ gate carries out the identity. Since the remaining two Hadamard operations cancel one another, the overall result for $a = 0$ is the identity. The action of a controlled-$Z$ gate which is preceded and succeeded by a Hadamard gate acting on the target is therefore equal to that of a CNOT for which the role of the control and target qubits are unchanged (once again, this is shown in Fig. 1.5). We say that such gates are equal up to single-qubit rotations, or locally equivalent.

Another entangling two-qubit gate, one that we will encounter several times in the main part of this thesis, is named the controlled-phase gate. This gate multiplies all states in the standard two-qubit basis by the identity, with the exception of the state with $ab = 11$ which is multiplied by a phase factor of $e^{i\phi}$. The corresponding matrix representation of a controlled-phase gate in the standard two-qubit basis is therefore given by

$$U_{\text{controlled-phase}}(\phi) = \begin{pmatrix} 1 \\ 1 \\ 1 \\ e^{i\phi} \end{pmatrix}.$$  \hfill (1.11)

For the special case of $\phi = \pi$ this gate is equal to a controlled-$Z$ gate [see Eq. (1.9)] and thus locally equivalent to CNOT. Furthermore, note that for the special case of $\phi = 0$ (or, equivalently, $\phi = 2\pi$) it is not an entangling gate as it then carries out the identity operation.
Above we showed that CNOT and controlled-Z are locally equivalent and the single-qubit rotation that turns one gate into the other is a Hadamard gate. In the general case the single-qubit rotations that map a given two-qubit gate to another may be nontrivial to determine. One is, however, often confronted with the question whether or not a given set of two-qubit gates are locally equivalent. To this purpose, Makhlin identified a set of numbers that are invariant under single-qubit rotations preceding or succeeding a two-qubit gate [68]. These so-called Makhlin invariants, which can be calculated straightforwardly, can then be used to answer the question of equivalence of two-qubit gates.

We also point out that there are entangling two-qubit gates that cannot be described as the controlled-operation gates discussed above. As an important example, we quickly describe the √SWAP gate. To derive the action of this gate, we begin with a SWAP gate, which is defined by swapping, or exchanging, the states of two qubits |a⟩ and |b⟩. Consequently, the states 00 and 11 are left unaltered while the states 01 and 11 are swapped. Its matrix representation in the ab = {00, 01, 10, 11} standard basis is therefore

\[ U_{\text{SWAP}} = \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{pmatrix}. \] (1.12)

The gate √SWAP is defined as a gate that squares to SWAP, and the corresponding matrix representation in the same standard two-qubit basis can thus be calculated to be

\[ U_{\sqrt{\text{SWAP}}} = \begin{pmatrix} 1 & e^{i\pi/4} & e^{-i\pi/4} & 0 \\ e^{-i\pi/4} & e^{i\pi/4} & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \] (1.13)

Note that neither this matrix nor the matrix of a SWAP gate in Eq. (1.12) is block-diagonal in the state of either qubit, as opposed to the matrices in Eqs. (1.5)-(1.9) which all belong to controlled-operation gates. Because of this, neither SWAP nor √SWAP is locally equivalent to any controlled-rotation gate (which is, of course, also reflected in a discrepancy of Makhlin invariants).

Finally, we combine the notions of qubits, single-qubit gates and two-qubit gates to visualize the concept of a quantum circuit. Figure 1.6 shows a generic circuit, consisting of an initialization, computation and measurement of four qubits labeled ‘1’ through ‘4.’ As shown, every single qubit is first initialized to the state |0⟩. During the computation, this particular circuit first applies a
Figure 1.6: Quantum circuit acting on four qubits. The circuit is divided into the three main parts corresponding to initialization, computation and measurement. Red boxes represent single bit gates, others are CNOT gates that act on two qubits.

single-qubit rotation to each qubit, then applies a CNOT gate the topmost two qubits (where qubit ‘1’ is the control qubit), then applies a single-qubit rotation to qubit 2 and CNOT to the lowermost two qubits, and so on. The fact that arbitrary single-qubit rotations and CNOT form a universal set of gates implies that arbitrary unitary operations can be enacted on any number of qubits in the same fashion as it is done in Fig. 1.6.

1.2.3 Quantum Parallelism: Search Algorithm due to Grover

The great power of quantum computation is rooted in the fact that the qubit Hilbert space is exponentially large in the number of present qubits. Assume we have a pair of qubits in the state $|0\rangle \otimes |0\rangle$ and enact a Hadamard gate [see Fig. 1.4(a)] on each qubit, resulting in

$$
(H \otimes H) (|0\rangle \otimes |0\rangle) = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)
$$

$$
= \frac{1}{2}(|00\rangle + |01\rangle + |10\rangle + |11\rangle).
$$

This state describes an equal superposition of four quantum states which can be taken to encode the numbers 0, 1, 2 and 3 in binary. Similarly, if we start with a set of $n$ qubits initialized to the state $|0\rangle \otimes |0\rangle \otimes \ldots \otimes |0\rangle = (|0\rangle)^\otimes n$ and again enact a Hadamard gate on each qubit, we obtain an equal superposition of exponentially many quantum states within the $N = 2^n$ dimensional Hilbert space,

$$
H^\otimes n |0\rangle^\otimes n = \frac{1}{\sqrt{N}} \sum_x |x\rangle,
$$

(1.16)
where, as in Eq. (1.15), the sum is over all \( N \)-many binary numbers \( x \) that range from 0 to \( 2^n - 1 \). Because of this superposition, the action of any quantum gate acting on any of these qubits will alter exponentially many coefficients in parallel. However, while one can evaluate a quantum gate for exponentially many values in a single step it is impossible to read out this exponential information stored in the \( n \)-qubit Hilbert space because, at the end of the quantum circuit, we can only measure the states of \( n \) qubits. It is therefore a nontrivial task to design quantum algorithms that allow one to make use of quantum parallelism. In Sec. 1.1.2 we have pointed out that Grover’s algorithm, among others, provides an example of how to make use of the exponentially large qubit Hilbert space.

We now take a look at the principle of Grover’s search algorithm [9], which can be used to search a large database of a total of \( N \) items, denoted by \( x \), for a single particular entry, \( \bar{x} \). Assume we are given a boolean-valued truth function \( t(x) \) which is equal to 1 if \( x \equiv \bar{x} \) is the entry we are looking for, and \( t(x) = 0 \) otherwise. In other words, this truth functions \( t(x) \) can be defined as

\[
t(x) = \begin{cases} 
1 & \text{if } x \equiv \bar{x} \\
0 & \text{otherwise.}
\end{cases} 
\]  

(1.17)

On a classical computer one would have to evaluate this function \( t(x) \) value by value, until \( t(x) = 1 \) is found. On average, this will take at least \( N/2 \) calls of this function \( t(x) \).

On the contrary, as we show now, this can be done in \( O(\sqrt{N}) \) computation steps on a quantum computer. Figure 1.7(a) illustrates, by means of a generic function \( f(x) \), two operations that we use to explain Grover’s algorithm. In case of the first operation, called phase inversion, the function value \( f(\bar{x}) \), for some \( \bar{x} \), is multiplied by -1 while all other values of this function remain unchanged. The other operation is called inversion about the mean, where the mean value is denoted by \( \mu \). Since the difference between \( f(x) \) and \( \mu \) is \( f(x) - \mu \), the function \( f(x) \) gets mapped to \( \mu - [f(x) - \mu] = -f(x) + 2\mu \). Efficient quantum circuits for these two operations are given in Ref. [66].

With these two relatively simple operations in hand we can now describe Grover’s algorithm. To do this, we first need \( n \) qubits that are used to encode \( 2^n = N \) numbers by forming the superposition (1.16). We can then identify the amplitude of every state \( |x\rangle \) in Eq. (1.16) as a constant function, \( f(x) = \frac{1}{\sqrt{N}} \), which is shown in the topmost plot in Fig. 1.7(b). As also shown in this figure, we begin Grover’s algorithm by applying phase inversion onto this function \( f(x) = \frac{1}{\sqrt{N}} \), where \( t(\bar{x}) \equiv 1 \)
Figure 1.7: Basics on Grover’s search algorithm. (a) Demonstration of phase inversion (left) and inversion about the mean (right) on the basis of a real function \( f(x) \) (see main text). (b) We identify the distribution of phase factors in Eq. (1.16) as a function \( f(x) = \frac{1}{\sqrt{N}} \) (topmost plot). As described in the text, Grover’s algorithm begins by applying phase inversion yielding the function \( g(x) \) (middle plot) defined in Eq. (1.19), and then proceeds by applying inversion about the mean (lowermost plot).

Defined in Eq. (1.17) determines the value \( \bar{x} \) for which the phase gets inverted. In other words, we carry out the mapping

\[
\frac{1}{\sqrt{N}} \sum_x |x\rangle \rightarrow \frac{1}{\sqrt{N}} \sum_{x \neq \bar{x}} |x\rangle - \frac{1}{\sqrt{N}} |\bar{x}\rangle = \frac{1}{\sqrt{N}} \sum_x (-1)^{t(x)} |x\rangle,
\]

where in the last step we used the fact that \( t(\bar{x}) = 1 \) and \( t(x) = 0 \) otherwise. The quantum circuit of Ref. [66] for this operation only needs to query the function \( t(x) \) once. The function \( f(x) = \frac{1}{\sqrt{N}} \) is thereby mapped to a new function, denoted \( g(x) \), which takes the values

\[
g(x) = \begin{cases} 
-\frac{1}{\sqrt{N}} & \text{if } x = \bar{x} \\
\frac{1}{\sqrt{N}} & \text{otherwise.} 
\end{cases}
\]

and is shown in Fig. 1.7(b) in the middle plot. Again referring to Fig. 1.7(b), we then carry out an inversion about the mean. Note that the mean value is just below \( \frac{1}{\sqrt{N}} \), so the result of inverting \( g(x) \) about the mean value \( \mu \approx \frac{1}{\sqrt{N}} \) changes the value of \( g(\bar{x}) \) which gets mapped to approximately \(-g(\bar{x}) + 2\mu = \frac{3}{\sqrt{N}}\), while all other values of \( g(x) \) remain almost unchanged. By applying the steps
of phase inversion and inversion about the mean we have thus effectively enhanced the amplitude of the state $|\bar{x}\rangle$ in Eq. (1.16) by $2\mu = \frac{2}{\sqrt{N}}$.

Grover's algorithm then proceeds by iterating these two steps of phase inversion and inversion about the mean. To an initially good approximation, the mean value can be taken as a constant at $\mu \simeq \frac{1}{\sqrt{N}}$, and so with the next iteration the amplitude of $|\bar{x}\rangle$ in Eq. (1.16) increases again by $2\mu \simeq \frac{2}{\sqrt{N}}$ from $\frac{3}{\sqrt{N}}$ to $\frac{5}{\sqrt{N}}$, and with the next iteration it increases to roughly $\frac{7}{\sqrt{N}}$, and so on. However, since the mean $\mu$ decreases slowly with every iteration [as we see in the first step in Fig. 1.7(b)] the change of the amplitude of $|\bar{x}\rangle$ actually slightly decreases with each iteration. Nonetheless, upon carrying out many iterations the maximum value of this amplitude approaches 1 (up to a minor correction that depends on $N$). This concludes Grover's algorithm.

To be able to make a quantitative statement of how many of the iterations shown in Fig. 1.7(b) need to be carried out, let us consider the case where the amplitude of the state $|\bar{x}\rangle$ has reached the value $1/\sqrt{2}$. If we then measure the $n$-qubit state [which was initialized to the superposition (1.16)] we will find the desired value, $\bar{x}$, with probability $(1/\sqrt{2})^2 = 1/2$. How many iterations does it take before the amplitude in question turns to $1/\sqrt{2}$? This is easy to evaluate if we assume that the mean value stays constant at $\mu = \frac{1}{\sqrt{N}}$. From the discussion above, we can conclude that after $s$ iterations the amplitude is given by $\frac{2s+1}{\sqrt{N}}$, and setting this equal to $1/\sqrt{2}$ yields $s \approx \sqrt{N}/(2\sqrt{2}) \sim \sqrt{N}$. Taking into account that the mean value is not constant with each iteration slightly increases the number of iterations by a constant factor, and one will find that the important result that Grover’s algorithm only requires $O(\sqrt{N})$ iterations indeed holds [9].

We have thus seen how a quantum computer may, in principle, gain computational power over classical computation. In fact, Grover’s algorithm has been successfully implemented in small-scale experiments in the late 1990s [69, 70, 71], however, in order to show the asymptotic quadratic speedup significantly large numbers of qubits are needed. Note that for large-scale computers and much longer computations the quantum information stored by qubits needs to be successfully protected using some kind of quantum error correction. A demonstration of how such a correction can be implemented follows in the subsequent section.

**1.2.4 Quantum Error Correction**

We have just seen how one may in principle gain computational power using a quantum computer. A rather important question looming ahead is, will we ever be able to make use of the
exponentially many degrees of freedom associated with the Hilbert space of qubits? Because, as mentioned above, quantum errors of arbitrarily small size will accumulate and spoil the computation unless they can be corrected. Errors stem from two major processes. First, imagine that in a real experiment we try to evolve a given Hamiltonian acting on a quantum two-level system encoding a qubit, in order to carry out a desired single-qubit rotation. Clearly, since the qubit state vector $\alpha|0\rangle + \beta|1\rangle$ is defined by the continuous variables $\alpha$ and $\beta$, the time-evolution of this Hamiltonian cannot be carried out exactly as desired. The same argument applies to the time evolution of Hamiltonians that carry out gates on multiple qubits, implying that all quantum gates will necessarily be subject to errors. Second, consider the case in which we let a qubit stay untouched for some amount of time, such as in a quantum memory. Here, the qubit will always be exposed to some unwanted interaction with the environment, leading to a process called decoherence.

Naively, one might be tempted to think that robustness in storing information can be achieved by copying the states of certain qubits to additional qubits at certain times during the computation process. These copies could be used at a later time if some part of the computation turns out to have failed. However, in the early 1980s an important contribution to the field of quantum information science was the formulation of the no-cloning theorem [72, 73], which states that copying unknown states is impossible. This theorem can be proved quickly by contradiction. Imagine there exists a unitary operation $U$ which copies the state of an arbitrary qubit $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ to a target qubit initialized to, say, $|0\rangle$. Its action can then be written as $U|\psi\rangle|0\rangle = |\psi\rangle|\psi\rangle = \alpha^2|0\rangle|0\rangle + \alpha\beta|0\rangle|1\rangle + \alpha\beta|1\rangle|0\rangle + \beta^2|1\rangle$. At the same time, linearity of the unitary operation $U$ implies that

\[
U|\psi\rangle|0\rangle = \alpha U|0\rangle|0\rangle + \beta U|1\rangle|0\rangle = \alpha|0\rangle|0\rangle + \beta|1\rangle|1\rangle \neq |\psi\rangle|\psi\rangle,
\]

unless $\alpha = 1$ or $\beta = 1$. This implies directly that such a unitary operation $U$, which would copy arbitrary qubit states, cannot have existed in the first place.

A crucial discovery that was made in the 1990s was the realization that while quantum errors appear to be continuous, they really are digital [10]. The basic idea behind this is that whenever an arbitrary single-qubit error $|\psi\rangle \rightarrow U_e|\psi\rangle$ occurs, then it can be projected into one of two
independent possible errors. Single-qubit errors are usually categorized as bit flips and phase flips which are described by the single-qubit operators $X$ and $Z$, respectively. The possible outcomes of this projection are then given by a unitary operation $U_e$ that is either the identity (corresponding to no error), or one of the operations $X$ (bit flip), $Z$ (phase flip) or $Y = XZ$ (both bit flip and phase flip). Here the matrix $Y$ is equal to the second Pauli matrix up to a proportionality factor, $Y = -i\sigma_y$.

Before being able to correct errors one first needs to be able to detect them. In classical computation, the simplest way to protect information in a magnetic hard drive is to store information that corresponds to a single “logical” bit, 0 or 1, by using three “physical” magnetic moments pointed along the same direction. For this repetition code, the logical states 0 and 1 are then given by 000 and 111, respectively. If one of these magnetic moments changes its direction due to thermal fluctuations, a measurement of all three bits then allows one to infer the correct logical bit state by a simple majority vote, and the flipped magnetic moment can subsequently be corrected. However, note that this type of error correction cannot be directly transferred to the quantum regime. This is because if we measure, in some basis, the state of a qubit that is initially in an unknown state, $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$, then this original qubit state will be projected onto one of the basis states and so the quantum information stored by the qubit will be lost.

So how can one detect and correct quantum errors without loss of information? The basic idea is, similar to classical code protection, to encode logical qubits into multiple physical qubits. Then, rather than measuring these “data” qubits directly, one first creates entanglement between the data qubits and additional, or “ancillary,” qubits. To determine if errors occurred one then measures these ancillas. To demonstrate this, consider an example of an error correcting code based on the classical three-bit repetition code described above. This code is capable to correct only one type of errors, which, as we demonstrate below, turn out to be $X$ errors.

In our example, we encode a qubit by representing logical basis states, $|0\rangle_L$ and $|1\rangle_L$, as states of three physical qubits so a general logical state is given by

$$|\psi\rangle_L = \alpha|0\rangle_L + \beta|1\rangle_L \equiv \alpha|0_10_20_3\rangle + \beta|1_11_21_3\rangle.$$  \hspace{1cm} (1.23)

These logical states are intrinsically better protected against logical bit flip errors than against phase flip errors. One way to see this is by identifying the corresponding logical operators for a bit
Table 1.1: Evaluation of a function that depends on the qubit pairwise parities measured
by the stabilizers $Z_1Z_2$ and $Z_2Z_3$ for the logical 3-qubit encoding described in the text.
For the case of no error the value of this function is equal zero. Otherwise, the result of
this function is an integer that denotes the qubit $i = 1, 2, 3$ that has undergone an $X_i$
error. A quantum circuit for evaluating the outcomes of the $Z_2Z_3$ stabilizer is shown in
Fig. 1.8.

<table>
<thead>
<tr>
<th>Three-qubit state</th>
<th>$(1 - Z_1Z_2)/2 + (1 - Z_2Z_3)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha \vert 010203 \rangle + \beta \vert 11213 \rangle$</td>
<td>0</td>
</tr>
<tr>
<td>$\alpha \vert 110203 \rangle + \beta \vert 011213 \rangle$</td>
<td>1</td>
</tr>
<tr>
<td>$\alpha \vert 011203 \rangle + \beta \vert 110213 \rangle$</td>
<td>2</td>
</tr>
<tr>
<td>$\alpha \vert 010213 \rangle + \beta \vert 111203 \rangle$</td>
<td>3</td>
</tr>
</tbody>
</table>

and phase flip which are given by, respectively, $X_L = X_1X_2X_3$ and $Z_L = Z_i$ (for any $i = 1, 2, 3$). If we can assume that errors are uncorrelated and multiple errors are therefore less likely to occur than a single error, then $X_L$ errors are obviously less likely than $Z_L$ errors.

Besides the three qubits that encode a single logical qubit, assume there is a fourth ancilla qubit which can be used to read out the parity of any pair of physical qubits. This parity is given by the eigenvalues of the operators $Z_1Z_2$, $Z_1Z_3$ and $Z_2Z_3$, known as stabilizers [74], where $Z_i$ acts on a physical qubit $i = 1, 2, 3$. However, only two of these stabilizers are linearly independent since $Z_1Z_2 = (Z_1Z_3)(Z_2Z_3)$. As long as no error occurs the parity of any pair, given by the eigenvalues of the corresponding stabilizers operator, is +1. We can quickly check this for, for example, the parity of the first and second qubit by enacting the stabilizer $Z_1Z_2$ on the correctly encoded state\(^8\) as given in Eq. (1.23),

$$Z_1Z_2 \langle \psi \rangle_L = Z_1Z_2 (\alpha \vert 0 \rangle_L + \beta \vert 1 \rangle_L)$$

$$= Z_1Z_2 (\alpha \vert 010203 \rangle + \beta \vert 11213 \rangle)$$

$$= \alpha \vert 010203 \rangle + (-1)^2 \beta \vert 11213 \rangle$$

$$= +1 \vert \psi \rangle_L.$$  (1.24)

Similarly, evaluating $Z_2Z_3$ will also yield an eigenvalue of +1. But, if we did a similar calculation for the operator $Z_1Z_2$ for a state where the first bit has flipped (or, it has undergone an $X_1$ error) we will find an eigenvalue of $-1$, while the eigenvalue of $Z_2Z_3$ will remain +1. In Table 1.1 we evaluate a function that depends on the measurement outcomes of the two stabilizers $Z_1Z_2$ and

\(^8\)As discussed in Sec. 1.2.1, the matrix representation of the $Z$ operator is given by $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ and so has eigenvalues +1 and $-1$ corresponding to the eigenstates $\vert 0 \rangle$ and $\vert 1 \rangle$, respectively.
Figure 1.8: Quantum circuit acting on four physical qubits for parity check operator $Z_2Z_3$ for two of the three physical qubits belonging to a logical qubit that has been initialized to state $|\psi\rangle_L$. Besides $|\psi\rangle_L$ which is encoded into the qubits labeled 1 through 3, the ancilla qubit, labeled 4, is initialized to the state $|0\rangle_4$. As explained in the text, qubits 2 and 3 have the odd parity if the measurement projects the ancilla to be in state $|1\rangle_4$.

$Z_2Z_3$ for all four cases in which either one or none of the three physical qubits has undergone an $X$ error. As demonstrated in the table, the eigenvalues of these two stabilizers are sufficient to pinpoint which qubit, if any, is faulty (assuming at most one qubit has flipped).

Figure 1.8 shows a four-qubit quantum circuit that can be used to measure the stabilizer $Z_2Z_3$ (that is, the parity of qubits 2 and 3). This circuit comprises only two quantum gates, both of which are CNOT gates, and it begins with an initialization in which a logical qubit is encoded using the physical qubits 1 through 3, and the ancilla, qubit 4, is initialized to the state $|0\rangle_4$. As shown in the figure, this circuit could be used to ensure that the initialization of the qubit $|\psi\rangle_L$ resulted in a state that is truly of the form (1.23). So, in order to find out if the second and third qubit have even or odd parity, we first enact two CNOT gates for which the controls are qubits 2 and 3, and for both of which the target is the ancilla qubit. In the last step of this circuit we measure the state of the ancilla in the standard $\{|0\rangle_4, |1\rangle_4\}$ basis.

Before explaining the circuit itself in some detail, recall that, as introduced in Sec. 1.2.2, the result of enacting CNOT on a control qubit $|a\rangle$ and a target qubit $|b\rangle$ flips the state of the target if and only if the control is in state $a = 1$. Conferring with Eq. (1.6), if the control is in the state $|0\rangle + |1\rangle$ and the target is in one of the basis states, $|b\rangle$, the action of CNOT can then be written as

$$
(|0\rangle + |1\rangle)|b\rangle \xrightarrow{U_{\text{CNOT}}} |0\rangle|b\rangle + |1\rangle|b \oplus 1\rangle,
$$

where, as above, the $\oplus$ operator indicates addition modulo 2.
Let us now discuss the different possible measurement outcomes of the ancilla qubit at the end of the circuit shown in Fig. 1.8. If no error occurred during the initialization, the logical qubit is in a state $|\psi\rangle_L = \alpha|010203\rangle + \beta|111213\rangle$. The first CNOT shown in Fig. 1.8 acts on the control qubit 3 and target qubit 4. According to Eq. (1.25), this CNOT gate will then carry out the following map,

$$
(\alpha|010203\rangle + \beta|111213\rangle) |04\rangle \xrightarrow{U^{(1)}_{\text{cnot}}} \alpha|010203\rangle|04\rangle + \beta|111213\rangle|14\rangle.
$$

The second CNOT shown in Fig. 1.8 acts on the control qubit 2 and target qubit 4, and will thus carry out the map

$$
\alpha|010203\rangle|04\rangle + \beta|111213\rangle|14\rangle \xrightarrow{U^{(2)}_{\text{cnot}}} \alpha|010203\rangle|04\rangle + \beta|111213\rangle|04\rangle.
$$

The two CNOT operations therefore act as inverses of each other since qubits 2 and 3 have even parity. The resulting four-qubit state is then a product state of the logical qubit $|\psi\rangle_L$ and the ancilla qubit, and the measurement out of the ancilla yields $|04\rangle$ with eigenvalue $+1$.

This is in contrast to the case where during initialization qubit 3, for example, has erroneously flipped and the qubit is in a state outside the encoded space, $|\psi'\rangle_L = \alpha|010213\rangle + \beta|111203\rangle$. The first and second CNOT operations shown in Fig. 1.8 then act as follows:

$$
(\alpha|010213\rangle + \beta|111203\rangle) |04\rangle \xrightarrow{U^{(1)}_{\text{cnot}}} \alpha|010213\rangle|14\rangle + \beta|111203\rangle|04\rangle,
$$

and

$$
\alpha|010213\rangle|4\rangle + \beta|111203\rangle|04\rangle \xrightarrow{U^{(2)}_{\text{cnot}}} \alpha|010213\rangle|14\rangle + \beta|111203\rangle|14\rangle.
$$

In this case, the CNOT gates do not act as inverses of each other, yet still the final state is a product state of $|\psi'\rangle_L$ and the ancilla qubit. However, now the ancilla is in state $|14\rangle$, and its measurement yields eigenvalue $-1$ and thus an odd parity, indicating a bit flip error.

We note that in general when detecting errors, the logical qubit will be in a superposition of states $|\psi\rangle_L$ within the encoded space and states $|\psi'\rangle_L$ that have undergone an error. Assuming, for simplicity, that only one of the physical qubits has flipped, these states are then of the form $\sqrt{1-\epsilon^2}|\psi\rangle_L + \epsilon|\psi'\rangle_L$, with ideally small absolute values of $\epsilon$. Following the error detection steps discussed above will then entangle these leaked and non-leaked states with the ancilla qubit and the measurement of the ancilla will project the qubit state either into or out of the encoded space. Using Table 1.1 we can find out which, if any, qubit $i$ ($i = 1, 2, 3$) has flipped and in the case of an error one will apply an $X_i$ operation to map the qubit back into the encoded space.
Figure 1.9: Sketch of an experimental setup for three gate-defined quantum dots, each capturing a single electron.

This particular three-qubit repetition code has first been demonstrated as a proof of principle in 1998 for NMR quantum computation [75], and has later been implemented again for other schemes, for example by Reed et al. using superconducting qubits [76]. But, as we stated in the beginning, this type of error correction only allows for correcting $X$ errors, and so more involved schemes for error correction are required (see Sec. 1.1.3). Finally, we point out that a recent, comprehensive review over quantum error correction is given in Ref. [77].

1.3 Pulsing Heisenberg Exchange and Braiding Anyons

After having sketched the basic principles of various quantum computation proposals in Sec. 1.1.3, we now get to know the principle mechanisms for carrying out quantum gates in the two types of quantum computation which the main part of this thesis is about. First, in Sec. 1.3.1, we begin by discussing spin-based quantum computation. Here we show how one can control the exchange coupling $J$ which determines the strength of the Heisenberg exchange Hamiltonian $\mathcal{H} = J \mathbf{S}_1 \cdot \mathbf{S}_2$ acting on two spins. In Sec. 1.3.2, we then turn to quantum computation with non-Abelian anyons. In this case we illustrate the concept of how exchanging non-Abelian particles can be understood as braiding. Finally, Sec. 1.3.3 describes how the main part of this thesis is structured.

1.3.1 A Spin-Based Quantum Computer

As pointed out in Sec. 1.1.3, the ability to adiabatically switch on and off, or pulse, the isotropic exchange Hamiltonian, $J \mathbf{S}_1 \cdot \mathbf{S}_2$, between pairs of spin-1/2 particles is a promising resource for quan-
tum computation [41]. Such pulsed exchange has been demonstrated experimentally for electron spins in double quantum dots [42] as well as cold atoms trapped in optical lattices [78]. The exchange interaction is purely isotropic and so cannot change the total spin of the system it acts on and thus cannot be used to carry out arbitrary unitary operations. As a consequence, if logical qubits are represented by single spin-1/2 particles [41] or encoded into the singlet-triplet states of pairs of spin-1/2 particles [49], universal quantum computation requires additional resources beyond exchange (e.g., oscillating magnetic [43] or electric [79, 80, 81, 45] fields for single-spin qubits, and gradients in the Zeeman energy for two-spin qubits [42, 82, 83, 84]). However, if logical qubits are suitably encoded using three or more spin-1/2 particles then pulsed exchange alone is a sufficient resource for universal quantum computation [46, 47, 48].

Gate-defined semiconductor quantum dots with trapped electrons are promising systems for manipulating spin-1/2 particles [85]. Figure 1.9 shows such a device consisting of a semiconductor heterostructure, such as GaAs/AlGaAs or Si/Ge, which exhibits a two-dimensional electron gas (2DEG). A potential landscape affecting the electrons in the 2DEG can then be created using the metallic gates on top of the device, shown in gray in the figure. This potential can be chosen in such a way that most electrons get displaced from the entire region shown in the figure and only in certain regions, shown as blue circles, only a single electron remains. Each of these regions is called a gate-defined quantum dot.

Two images of such devices that were used in experiments are shown in Figs. 1.10(a) and (b) from a top view. As in Fig. 1.9, metallic gates, shown as thin structures, are placed on top of the semiconductor surface. For the double-quantum dot shown on in (a), we also plot the double-well potential $V(x)$ as a function of the horizontal $x$-direction as well as the wave functions associated with each electron occupying each quantum dot. Similarly, the potential of the triple-dot device shown in Fig. 1.10(b) describes a triple-well function as a function of the horizontal direction. The device in (b) was used in an experiment in which single-qubit operations were carried out [86] in the exchange-only quantum computation scheme considered in this thesis [46, 47, 48].

Figure 1.10(c) illustrates how one can pulse the Heisenberg exchange Hamiltonian $\mathcal{H} = J\mathbf{S}_1 \cdot \mathbf{S}_2$ between the two spins in the double quantum dot device of Fig. 1.10(a). This Hamiltonian depends on the exchange coupling, $J$, whose value is determined by the overlap of the two electron wave functions [87]. We assume $J = 0$ when the electrons are located far apart and the overlap is
Figure 1.10: Scanning tunneling microscope images of a semiconductor (a) double quantum-dot device [42] and a (b) triple quantum-dot device [86]. In (a), the electrostatic potential $V(x)$ of the double-quantum dot is also shown, including electron wave functions (shown in blue) that occupy the lowest energy level within each quantum well. (c) Pulsing, or turning on-and-off, the exchange Hamiltonian $H = J S_1 \cdot S_2$ between spins in a double quantum dot, such as that shown in (a).

negligible, as it is the case in the leftmost and the rightmost diagrams in Fig. 1.10(c) for a large tunnel barrier between the dots. However, if the tunnel barrier is decreased, as in the central diagram in (c), the overlap of the electron wave functions are longer negligible. By virtue of the Pauli exclusion principle, the two-fermion wave function will then energetically favor antiparallel spins, corresponding to a spin singlet state, over parallel spins, corresponding to a triplet state.\(^9\) Accordingly, the exchange coupling $J$, which denotes the energy difference between the singlet and triplet states, will take on a nonzero value. We therefore say that by decreasing (increasing) the voltage barrier, the Hamiltonian $J S_1 \cdot S_2$ is turned on (off). An exchange pulse of some duration $t$ can then be performed by going through the cycle of Fig. 1.10(c). Starting in the high-potential regime in which $J = 0$, one first transitions to the low-potential regime in which $J$ is finite and stays in this regime for the pulse duration $t$. Afterward, we transition back to the high-potential

\(^9\)We may calculate $J$ as a function of a tunneling matrix element $\tilde{t}$, which is assumed small compared to the charging energy, $U$, of a doubly-occupied dot, by casting this problem into the framework a simple two-site Hubbard model for two electrons. The corresponding Hamiltonian reads $H = U (n_{1,\uparrow} n_{1,\downarrow} + n_{2,\uparrow} n_{2,\downarrow}) - \tilde{t} \sum_{\sigma=\uparrow,\downarrow} (c_{2,\sigma}^\dagger c_{1,\sigma} + c_{1,\sigma} c_{2,\sigma}^\dagger) \equiv H^{(0)} + H^{(1)}$. Here we identify the first term as the unperturbed Hamiltonian since $\tilde{t}/U \ll 1$, with $c_{i,\sigma}^\dagger$ the creation operator of an electron in quantum dot $i$ with spin $\sigma$ and $n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}$ the number operator for dot $i$ and spin $\sigma$. If $\tilde{t} = 0$, the ground state energy for this Hamiltonian is equal to 0 and the energy of the first excited state, corresponding to a doubly-charged dot, is equal to $U$. For small values of $\tilde{t}$ it is easy to show that, due to the symmetry of the problem, the first-order contribution equals zero. In second order perturbation theory the ground state energy of the singlet is then lowered by $J \sim -\tilde{t}^2/U$, whereas the energy of the triplet is unchanged [87].
regime in which \( J = 0 \).

Of course, in actual experiments there will be anisotropic contributions to the Heisenberg exchange Hamiltonian, such as terms arising due to spin-orbit coupling or nuclear magnetic fields. We assume here that the isotropic Heisenberg interaction is the dominant term in the Hamiltonian, and that anisotropic effects are negligibly small. Most of these terms depend on the materials used in the semiconductor heterostructure. For example, the density of nuclear spins in silicon is significantly lower than in gallium arsenide [88, 89], a feature that leads to significantly longer coherence times of electron spins in silicon quantum dots [90].

The above procedure of manipulating individual spins is, from a practical point of view, significantly simpler than applying local magnetic fields [41] in order to manipulate individual spins. This is the main reason for the emergence of exchange-only spin quantum computing schemes that were initiated by Refs. [47, 48] soon after the original proposal due to Loss and DiVincenzo [41]. In Chapter 2 we present our work [91, 92, 93] on the explicit proposal of exchange-only quantum computation due to DiVincenzo et al. [46]. In this proposal, as described above and in Sec. 1.1.3, each qubit is encoded into the Hilbert space of three (or four) spin-1/2 particles and quantum gates are carried out by sequences of exchange pulses acting on pairs of spins. In this case, it is significantly more difficult to find pulse sequences for two-qubit gates than sequences for single-qubit gates. This is mainly because the Hilbert space of six spins, used to encode two qubits, has a much larger dimension than the Hilbert space of three spins that encode a single qubit. Our work constitutes results on how to analytically determine sequences of exchange pulses for two-qubit entangling gates.

### 1.3.2 A Topological Quantum Computer with Anyons

In topological quantum computation, particle-like excitations that obey non-Abelian statistics, known as non-Abelian anyons, are used to store and manipulate quantum information in an intrinsically fault-tolerant manner [52, 53, 51]. When \( n \) such particles are present, and held far enough apart, there is a degenerate Hilbert space with dimensionality exponentially large in \( n \). Distinct states in this Hilbert space cannot be distinguished by local measurements, but rather only by measurements over regions enclosing two or more particles. As sketched below, moving non-Abelian particles around one another can be viewed as braiding their worldlines in 2+1 dimensional space-time. In doing so, unitary operations are enacted on this degenerate Hilbert space which transform...
one ground state onto another. Provided the particles continue to be kept far enough apart as they are braided, the resulting unitary operation is identical for any two topologically equivalent braids and so is robust against errors.

Figure 1.11 illustrates how the result of interchanging non-Abelian anyons can be interpreted as a braid. Anyons, depicted by black and green circles, are spatially confined to a two-dimensional plane. When exchanging two neighboring particles we trace the worldlines of each particle as it moves through the corresponding 2+1 dimensional spacetime. The two different interchanges shown in Fig. 1.11(a) are the result of a clockwise exchange and a counterclockwise exchange. For ordinary particles these two operations are equivalent, because when exchanging a pair of bosons or fermions the two-particle wave function will simply acquire a factor of +1 or −1, respectively, independent of how this interchange is carried out. However, as we stated above, for anyons these two interchanges carry out nontrivial unitary operations $U_{cw}$ and $U_{ccw}$ onto the multi-dimensional Hilbert space. The two interchanges shown in the figure are, however, related in that they are inverses of each other, $U_{cw}^\dagger = U_{ccw}$.

In Fig. 1.11(b) a double clockwise interchange of two particles is shown in two different ways. For non-Abelian anyons the unitary operation enacted by such a double exchange, $U_{cw}^2$, is in general not proportional to the identity. On the left-hand side of Fig. 1.11(b), we view this interchange as a simple concatenation of two clockwise interchanges similar to those shown in (a). On the right-hand side in the same figure, this braid is shown in an equivalent representation by leaving the left-hand (black) particle fixed at its original position and moving the right-hand (red) particle around the fixed particle. A braid pattern of the latter type, in which in general for an arbitrary number of anyons only one is dragged around all others which remain at their fixed position, is a special type of braid that is called an “anyon weave.” In case of a weave, the mobile particle, called the “weft,” will usually be shown in red while the other particles, denoted as the “warp,” will be shown in black.

The two different braid patterns of Fig. 1.11(b) result in the same unitary operation, because the unitary operation corresponding to an anyon braid only depends on the braid’s topology. Any two braid patterns that can be continuously deformed into each other, without cutting a line and without interchanging the initial or final positions of the particles, result in the same unitary operation. Another example of this equivalence of braids is illustrated in Fig. 1.12 which shows
a first nontrivial example of a weave represented by two braids that can be deformed into one another. The diagram on the left represents idealized worldlines of particles that are being braided, while the diagram on the right could represent a braid that corresponds to a real experiment in which particles are subjected to perturbations from the environment.

Figure 1.12 highlights the important feature that the unitary operations corresponding to braids acted on the anyon Hilbert space are robust to local imperfections in the braid. This is in contrast to other quantum computing proposals in which the precise unitary operation of a desired quantum gate depends delicately on the precise physical implementation of the gate. For example, we learned in the previous section that in spin-based quantum computation certain gates can be carried out by pulsing the exchange interaction for some duration $t_0$. In a real experiment, this duration be of length $t_0\pm\delta t$ with some deviation $\delta t$ which ideally needs to be as small as possible. Such problems of inaccurate physical resources is not present in the case of topological quantum computation because the unitary operations due to braids do not depend on the braid details, as shown in Fig. 1.12.
Harmful errors can only occur, however, if perturbations act on more than one particle at a time. Such processes can be suppressed by keeping the anyons far apart from one another while being braided.

Fibonacci anyons are arguably the simplest non-Abelian particles for which, as already mentioned in Sec. 1.1.3, braiding alone is sufficient to carry out arbitrary quantum computations [53]. Unfortunately, these anyons appear to be much harder to realize experimentally than Majorana zero modes, for which braiding is not universal for quantum computation. Fibonacci anyons can in principle arise as quasiparticle excitations of the $k = 3$ Read-Rezayi state [56], which may describe the $\nu = 12/5$ fractional quantum Hall effect, as well as the $\nu = 2/3$ bosonic fractional quantum Hall effect in a rotating Bose condensate [94]. More recently it has been proposed that Fibonacci anyons might be engineered in systems in which charge $2e$ condensates formed by clusters of fractionalized excitations in Abelian quantum Hall fluids are induced via the proximity effect with ordinary superconductors [95, 96]. Fibonacci anyons can also appear as excitations of certain spin models [65] and related non-Abelian surface codes [64] with the potential to one day be realized experimentally [97, 98].

In Chapter 3 we present our work [99] on a quantum computing scheme in which Fibonacci anyons are used to store quantum information and all quantum gates are carried out solely by braiding [53]. Similar to spin-based exchange-only quantum computation in which qubits are en-
coded by three (or four) spin-1/2 particles, here each qubit is encoded by three (or four) Fibonacci anyons. Another similarity is that the problem of finding braid patterns for two-qubit gates are significantly harder to find than braids for single-qubit gates because, again, the Hilbert space of six (or eight) Fibonacci anyons encoding two qubits is much larger than that of three (or four) anyons that encode only a single qubit.

A significant difference between spin-based and Fibonacci-anyon based quantum computation is, however, that in the case of braiding with anyons there does not seem to exist a finite braid for carrying out exact entangling two-qubit gates (this curiosity has been commented on in Ref. [100]). Because of this, the only known two-qubit gate braids approximate two-qubit gates and it is a nontrivial problem to establish methods for finding or generating braids that approximate two-qubit gates to an arbitrary degree. This is the problem that we take on in Chapter 3.

1.3.3 Structure of the Main Part of this Thesis

We have now gotten to know the mechanisms for carrying out quantum gates in the two quantum computing proposals that we are going to focus on in the remainder of this thesis. The remainder of this thesis is organized as follows.

In Chapter 2, we consider a spin-based quantum computer in which qubits are encoded using three or four spin-1/2 particles. In Secs. 2.1 and 2.2, we begin by discussing how in exchange-only spin-based quantum computation single-qubit rotations and two-qubit quantum gates can be carried out by pulsing the Heisenberg exchange Hamiltonian. We then address the problem of constructing pulse sequences for carrying out two-qubit quantum gates. Before our work, this problem has, due to its complexity, only been solved using numerical search techniques.

In Sec. 2.3, we present the first analytical construction of a set of two-qubit gate pulse sequences, yielding a family of entangling two-qubit quantum gates [91]. A similar two-qubit gate pulse sequence construction, which uses new elements in addition to those of the construction of Sec. 2.3, is presented in Sec. 2.4 [93]. The pulse sequences yielded by the latter construction are significantly shorter than the sequences of the former construction. Both of the sequences of Secs. 2.3 and 2.4 can be used to carry out a controlled-phase gate (see Sec. 1.2.2) for which the phase can be freely chosen by adjusting the underlying pulse sequence.

Section 2.5 then gives an analytic derivation [92] of the best known two-qubit gate pulse sequence, which had previously been found by Fong and Wandzura through a numerical search [101].
As a part of this derivation, we categorize the Fong-Wandzura sequence as being the shortest and thus most efficient sequence within an infinite class of two-qubit gate pulse sequences.

Next, in Chapter 3, we consider a topological quantum computer in which either three or four Fibonacci anyons are used to represent a qubit. In Secs. 3.1 and 3.2 we first introduce the Fibonacci anyon model and explain in detail how to carry out unitary operations on the Hilbert space of anyons by braiding. In the rest of Chapter 3 we then present a new method for finding two-qubit braid patterns [99].

The braids used in our two-qubit gate constructions are based on a particular kind of three-anyon braids that were first used by Reichardt and can be generated by using a particular iteration equation [102]. Section 3.3 describes in detail how these braids may be generated. Sections 3.4 and 3.5 then describe how these three-anyon braids can be implemented in two explicit two-qubit braid constructions to generate entangling two-qubit braids.

To close this Dissertation, in Chapter 4 we summarize our work and then discuss open problems in the two fields of quantum computation that were considered.
CHAPTER 2

TWO-QUBIT GATE PULSE SEQUENCES FOR A SPIN-BASED QUANTUM COMPUTER

2.1 Introduction to Exchange-Only Quantum Computation

In the introductory chapter we stated that in spin-based quantum computation the ability to turn on-and-off, or pulse, the Heisenberg exchange Hamiltonian \( J \mathbf{S}_1 \cdot \mathbf{S}_2 \) between pairs of spin-1/2 particles is a useful tool for manipulating quantum information. If this isotropic exchange is the only resource for carrying out quantum logical operations, qubits need to be encoded into the Hilbert space of at least three spin-1/2 particles [47, 48]. In Sec. 1.3.1 we considered the common experimental realization of spin-based quantum in which spins of electrons, captured in gate-defined semiconductor quantum dots, are used to represent qubits. In that section we illustrated the concept of an exchange pulse and how it can be performed by changing the potential landscape that confines electrons by voltage biasing through metallic gates.

DiVincenzo et al. [46] presented the first explicit scheme for carrying out universal quantum computation using only pulsed exchange. In this scheme, each qubit is encoded into the two-dimensional Hilbert space of three spin-1/2 particles with total spin fixed to be 1/2 and polarized along a given direction. For a linear array of spin-1/2 particles, arbitrary single-qubit rotations can then be carried out by performing a sequence of up to four exchange pulses between nearest-neighbor spins within a given encoded qubit.

In Sec. 1.3.1, Fig. 1.9 shows a schematic experimental setup of a semiconductor quantum dot device. The experimental progress on the implementation of such triple-dot devices used for exchange-only qubits, as it has been proposed in Ref. [46], has been remarkable [103, 44, 104, 105, 86, 106]. A related scheme, based on the so-called resonant exchange qubit [107], in which the exchange interactions between spins within the qubit are kept “always on” (see also Ref. [108]) has also recently been demonstrated [109]. These resonant exchange qubits offer resistance to leakage out of the encoded qubit space and the possibility for carrying out two-qubit gates with a single exchange pulse [110]. In the present work we adopt the three-spin qubit encoding for exchange-only quan-
tum computation of Ref. [46] and assume that the exchange interaction between spins is completely switched off except when pulsing. In this case two-qubit gates require nontrivial sequences of many exchange pulses to avoid leakage out of the encoded space [46, 111, 112, 101, 90, 113, 91].

By performing a numerical search, DiVincenzo et al. [46] were able to find a sequence of 19 nearest-neighbor exchange pulses for a linear array of spins which carries out a two-qubit gate locally equivalent to a controlled-\textsc{not} (\textsc{cnot}) gate (i.e., a \textsc{cnot} gate up to single-qubit rotations) on two three-spin qubits. This numerically obtained sequence was later confirmed to be exact [112]. As we stated in the introduction in Sec. 1.2.2, the set of single-qubit rotations and \textsc{cnot} gates is a standard universal gate set for quantum computation, and so these pulse sequences can be used to perform any quantum algorithm [66].

A key requirement in the \textsc{cnot} construction of Ref. [46] is that the total spin of all six spin-1/2 particles forming the two encoded qubits acted on by the gate must be 1. As pointed out in the same reference, for electron spins this condition can be forced by initializing the qubits in an external magnetic field. This total spin requirement cannot be relaxed, because if the total spin of all six particles is 0 then the 19-pulse sequence does not result in the same two-qubit gate and, in fact, leads to leakage out of the encoded qubit space.

More recently, Fong and Wandzura [101] found a sequence of nearest-neighbor exchange pulses, again for a linear array of spins, which performs the same two-qubit gate (also locally equivalent to \textsc{cnot}) in both the total spin 0 and total spin 1 sectors. Remarkably, with 18 pulses, this sequence is shorter than the 19-pulse sequence of Ref. [46]. Although this sequence was obtained by numerical minimization of a cost function using a genetic algorithm, the final result is exact and has a particularly elegant form consisting of $\sqrt{\textsc{swap}}$, inverse $\sqrt{\textsc{swap}}$, and \textsc{swap} pulses. Related two-qubit gate sequences with fewer pulses (16 and 14) have since been found for geometries other than linear arrays of spins [114].

In the present chapter, we present the result of our work on the field of exchange-only spin quantum computation. Section 2.2 describes how we describes states in the Hilbert of spin-1/2 particles, and introduces the qubit encoding of Ref. [46]. In Sec. 2.3 we give an analytical construction of a sequence of 39 exchange pulses [91]. An earlier version of this construction, together with a display of alternative pulse sequences of the same length, has been published in Ref. [115]. Section 2.4 then gives another construction that is similar to the one of Sec. 2.3 but yields sequences that
are comprised of only 25 pulses [93] rather than 39 pulses. Yet, both sequences of Secs. 2.4 and 2.3 can be used to carry out the same two-qubit gates. Afterward, in Sec. 2.5 we provide an analytic and intuitive derivation on the Fong Wandzura sequence. Finally, we present our conclusions in Sec. 2.6.

### 2.2 Hilbert Space and Three-Spin Qubit Encoding

Because the isotropic exchange interaction between pairs of spin-1/2 particles is rotationally invariant, any unitary operation carried out purely by pulsing this interaction can be described entirely in terms of total spin quantum numbers, with no reference to $S_z$ quantum numbers.

Figure 2.1(a) illustrates a notation which exploits this fact. This notation is inspired by that used in Refs. [58, 116] for non-Abelian anyons when finding braiding patterns for topological quantum computation, a problem closely related to that of finding pulse sequences for exchange-only quantum computation. Here, spin-1/2 particles are represented by solid dots enclosed in ovals labeled by the total spin of the enclosed particles. Any choice of non-intersecting ovals for which each oval encloses two particles, two ovals, or one of each, amounts to a basis choice. The basis states correspond to all possible labelings of ovals consistent with the triangle rule for adding spin quantum numbers. When referring to these basis states in the text we will use parentheses to
represent ovals so, e.g., the state shown in Fig. 2.1(a) would be written \(((\bullet)_{1}(\bullet\bullet)_{0})_{1/2}\) where the symbol • denotes a spin-1/2 particle. It is always possible to change bases from one set of ovals to another by using the appropriate spin recoupling coefficients.\(^1\)

A multi-spin state with total spin \(S\) (i.e. the label of the oval enclosing all the particles is \(S\)) has a \((2S + 1)\)-fold degeneracy associated with the possible values of the \(S_z\)-component. However, as emphasized above, all spin operations we consider for exchange-only quantum computation are rotationally invariant, so at no point will it be necessary to refer to these \(S_z\) quantum numbers. In what follows we will therefore treat states like • or (••)\(_1\) as single states in Hilbert space, even though when the \(S_z\) degeneracy is counted they are twofold and threefold degenerate, respectively.

To carry out exchange-only quantum computation it is necessary to use suitably encoded logical qubits \([47]\). The basis states for the three-spin qubit encoding of Ref. \([46]\) are shown in Fig. 2.1(b). In this encoding, the logical qubit states are those with total spin 1/2, with the logical \(|0_L⟩\) and logical \(|1_L⟩\) corresponding, respectively, to the states for which two of the particles are in a singlet or a triplet. The choice of the two particles whose total spin determines the state of the logical qubit is, of course, purely a basis choice. The price one pays for this qubit encoding is that there is a noncomputational state, denoted \(|nc⟩\) in Fig. 2.1(b), in which the total spin of the three particles is 3/2.

Transitions from the computational space to the noncomputational space are known as leakage errors. When carrying out single-qubit rotations by pulsing the exchange interaction within a given encoded qubit, the total spin of that qubit is unchanged and there are no leakage errors. However, carrying out two-qubits gates requires some pulses that act on spins from each qubit. Such pulses alter the total spin of each encoded qubit and thus induce transitions into the noncomputational space. It is therefore a nontrivial problem to determine pulse sequences which carry out leakage-free entangling two-qubit gates.

Figure 2.2(a) shows two logical qubits each of which has total spin 1/2, so the total spin of all six spin-1/2 particles, labeled \(g\), can be either 0 or 1. In our construction we assume these spins form a linear array and only consider nearest-neighbor exchange pulses. The choice of qubit bases in the figure is convenient for our two-qubit gate construction. The full Hilbert spaces of the \(g = 0\)

\(^1\)Since we do not use wave functions written explicitly in terms of \(S_z\) quantum numbers it is necessary to specify a phase convention for states labeled only by total spin quantum numbers. We take this convention to be the standard Condon-Shortley phase choice. This choice also determines the phases of the relevant spin-recoupling coefficients. It is because these coefficients are real-valued that all pseudospin rotation axes in our construction lie in the \(xz\)-plane.
and $g = 1$ sectors are five- and nine-dimensional, respectively, where, as described above, we ignore the $S_z$ degeneracy. The set of unitary operators acting on this space is then $SU(5) \oplus SU(9)$, once irrelevant overall phase factors are removed. The number of independent parameters appearing in these unitary operators are $24 = 5^2 - 1$ (for $g = 0$) and $80 = 9^2 - 1$ (for $g = 1$). It is because of the enormous size of these high-dimensional search spaces that all previous work finding pulse sequences for two-qubit gates has been numerical, even when the result has the elegant form of the Fong-Wandzura sequence.

### 2.3 Construction of a 39-Pulse Sequence

In this section we construct a family of sequences consisting of 39 nearest-neighbor exchange pulses on a linear array of spins which perform entangling two-qubit gates on three-spin qubits, including a gate which is locally equivalent to CNOT [91]. The main new feature of our construction is that it can be carried out purely analytically, requiring at most the solution of a transcendental equation in one variable. Unlike the 19-pulse sequence of Ref. [46], but like the 18-pulse sequence of Fong and Wandzura,[101] the action of our 39-pulse sequences are independent of the total spin of the two encoded qubits. Indeed, we point out that any pulse sequence which carries out
Figure 2.3: Exchange pulse between two spin-1/2 particles, represented by a double arrow labeled by the pulse duration $t$ defined in the text, which produces the operation $U_2(t)$. In the basis $a = \{0, 1\}$, the matrix representation of $U_2(t)$ is a $z$-axis rotation in pseudospin space with $\uparrow = (\bullet)\_0$ and $\downarrow = (\bullet)\_1$.

A leakage-free two-qubit gate in the total spin-1 sector while acting on only five of the six spins needed to encode the qubits (which is the case for our sequences, as well as those found by Fong and Wandzura[101] and in Ref. [114], but not for the sequence of Ref. [46] which acts on all six spins) will perform the same two-qubit gate in the total spin-0 sector. Using such sequences eliminates the need to initialize encoded qubits in a magnetic field.

An outline of our analytic approach to constructing pulse sequences is illustrated in Fig. 2.2(b). After establishing the fundamental resource — the exchange interaction between two spin-1/2 particles — we consider the Hilbert spaces of three spins, four spins, and finally five spins. At each stage of our construction we work with a restricted set of operations which allows us to work entirely in effective Hilbert spaces which are at most two-dimensional, i.e. that of a spin-1/2 pseudospin. The space of operations is then that of simple three-dimensional rotations and this allows us to use geometric intuition to analytically determine the required pulse sequences.

Our construction results in a controlled-phase gate which is diagonal in the $ab$ basis for the two qubits shown in Fig. 2.2(a) and which applies a phase factor of $e^{-i\phi}$ to the state with $ab = 11$ while multiplying the states $ab = 00, 01,$ and 10 by 1. We are able to set $\phi$ to any desired phase and the case $\phi = \pi$ yields a gate which is locally equivalent to CNOT. Two examples of the resulting pulse sequences, which consist of 39 pulses and either one or two single-qubit rotation pulses, are given in Sec. 2.3.6.

2.3.1 Two Spins

We begin our construction by considering an exchange pulse between two nearest-neighbor spins (e.g., the spins circled in Fig. 2.2(b) in the diagram labeled “Two Spins”). Figure 2.3 illustrates the effect of such a pulse generated by applying the Hamiltonian $JS_1 \cdot S_2$ for a time measured in $1/J$.
\( \hbar = 1 \) whose product is then given by the dimensionless duration \( t \).\(^2\) The matrix representation of the resulting unitary operation in the \((\bullet\bullet)\) basis with \( a = \{0, 1\} \), i.e. the singlet-triplet basis where, as described in the previous section, we ignore the \( S_z \) degeneracy, is

\[
U_2(t) = e^{-it(S_1 \cdot S_2 + \frac{3}{4})} = \begin{pmatrix} 1 \\ e^{-it} \end{pmatrix} e^{-it/2} e^{it2 \cdot \sigma/2}.
\tag{2.1}
\]

Here \( \sigma = (\sigma_x, \sigma_y, \sigma_z) \) is the Pauli vector and the additive constant \( 3/4 \) in the exponent gives a convenient choice for the irrelevant overall phase factor. If we view the states \((\bullet\bullet)0\) and \((\bullet\bullet)1\) as the \( \uparrow \) and \( \downarrow \) states, respectively, of a pseudospin then this operation is a \( z \)-axis rotation in pseudospin space through the angle \( t \) multiplied by a phase factor.

Our convention throughout will be that positive pseudospin rotation angles correspond to left-handed rotations about the given axis (i.e., a rotation through angle \( t \) about an axis \( \hat{n} \) corresponds to the \( SU(2) \) operation \( U = e^{it\hat{n} \cdot \sigma/2} \)). The duration of each pulse is positive and can always be taken to be in the range \( 0 < t < 2\pi \). For the inverse of an exchange pulse of duration \( t \) we pulse for duration \( s = 2\pi - t \).

### 2.3.2 Three Spins

Figure 2.4 shows the action of two different nearest-neighbor exchange pulses on the Hilbert space of three spin-1/2 particles (e.g., the three spins circled in Fig. 2.2(b) in the diagram labeled “Three Spins”). As described in Sec. 2.2, the choice of labeled ovals corresponds to a particular basis choice. The three-spin basis shown in Fig. 2.4 consists of the states \((\bullet\bullet\bullet)\) where \( ac = 0, 1, 2, 11, \) and \( 13 \). For clarity, when referring to vertically aligned spins in a given figure the convention is that topmost in the figure corresponds to leftmost in the text.

Matrix representations of the unitary operations produced by the exchange pulses are also shown in Fig. 2.4. These matrices are expressed in the \((\bullet\bullet\bullet)\) basis with \( ac = \{0, 1, 2, 11, 13\} \) and consist of a \( 2 \times 2 \) block acting on the total spin \( c = 1/2 \) sector and a phase factor multiplying the \( c = 3/2 \) state.

We describe the two-dimensional \( c = 1/2 \) sector in terms of a pseudospin with \( \uparrow = ((\bullet\bullet)0\bullet)_{1/2} \) and \( \downarrow = ((\bullet\bullet)1\bullet)_{1/2} \). The unitary operations shown in Fig. 2.4 are then pseudospin rotations about two different axes. Pulsing the top two spins results in an operation that is diagonal in \( a \) and hence

---

\(^2\)Actual pulses will not simply involve switching on and off a constant exchange coupling \( J \), and the dimensionless pulse duration \( t \) is more accurately taken to be the time integral of a time-dependent \( J \) over the pulse. For our choice of units, \( t = \pi \) corresponds to a two-spin SWAP operation.
Figure 2.4: Nearest-neighbor exchange pulses (denoted $U_2$ in the text) and their matrix representations in the $ac = \{0\frac{1}{2}, 1\frac{1}{2}| 1\frac{3}{2}\}$ basis. Each $3 \times 3$ matrix is block-diagonal, consisting of a $2 \times 2$ sector with $c = 1/2$ and a one-dimensional sector with $c = 3/2$. In the $c = 1/2$ sector the pulses produce rotations about either $\hat{z}$ or $\hat{n}_1 = (-\sqrt{3}/2, 0, -1/2)$ for a pseudospin where $\uparrow = (\bullet\bullet)_0\frac{1}{2}$ and $\downarrow = (\bullet\bullet)_1\frac{1}{2}$.

is a rotation about the $z$-axis. In the $((\bullet\bullet)_a\bullet)_{1/2}$ basis with $a = \{0, 1\}$, the matrix representation of this operation is the same as that given in (2.1).

Likewise, the matrix representation of an exchange pulse between the bottom two spins (see Fig. 2.4) in the $((\bullet\bullet)_{a'})_{1/2}$ basis with $a' = \{0, 1\}$ is

$$U_{2,a'}^{c=1/2}(t) = \begin{pmatrix} e^{-it/2} e^{it\hat{z}\cdot \sigma/2} & 0 \\ 0 & e^{-it} \end{pmatrix} = e^{-it/2} e^{it\hat{z}\cdot \sigma/2}. \quad (2.2)$$

Here the notation $U_{2,a'}^{c=1/2}$ indicates the matrix representation of $U_2$ (in this case the unitary operation produced by pulsing the exchange interaction between the bottom two spins) in the $a'$ basis in the sector with total spin $c = 1/2$. To find the matrix in the original $((\bullet\bullet)_a\bullet)_{1/2}$ basis we perform the basis change

$$((\bullet\bullet)_a\bullet)_{1/2} = \sum_{a'} F_{1,aa'} ((\bullet\bullet)_{a'})_{1/2}, \quad (2.3)$$

where the matrix elements

$$F_{1,aa'} = \langle (\bullet\bullet)_{a'} | ((\bullet\bullet)_a\bullet)_{1/2} \rangle \quad (2.4)$$

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are recoupling coefficients for three spin-1/2 particles with total spin 1/2. \( F_{1,aa'} \) can be expressed as a 2 × 2 matrix which transforms from the \( a' = \{0, 1\} \) basis to the \( a = \{0, 1\} \) basis,

\[
F_1 = \begin{pmatrix}
-1/2 & \sqrt{3}/2 \\
\sqrt{3}/2 & 1/2
\end{pmatrix} = \hat{f}_1 \cdot \sigma,
\]

where \( \hat{f}_1 = (\sqrt{3}/2, 0, -1/2) \). The action of pulsing the exchange interaction between the bottom two spins in the \((\circ \circ)_a \circ \circ)_{1/2} \) basis with \( a = \{0, 1\} \) is then

\[
U_{2,a}^{c=1/2}(t) = F_1 U_{2,aa'}^{c=1/2}(t) F_1 = e^{-it/2} e^{it\hat{n}_1 \cdot \sigma/2},
\]

where \( F_1 = F_1^\dagger \). The rotation axis \( \hat{n}_1 = 2\hat{f}_1 (\hat{f}_1 \cdot \hat{z}) - \hat{z} = (-\sqrt{3}/2, 0, -1/2) \) makes an angle \( \cos^{-1} \hat{n}_1 \cdot \hat{z} = -\frac{2\pi}{3} \) with the \( z \)-axis, as shown in Fig. 2.4.

The \( c = 3/2 \) sector consists of a single state which can be expressed equivalently either as \((\circ \circ)_1 \circ \circ)_{3/2} \) or \((\circ \circ)_1 \circ \circ)_{3/2} \). Consulting (2.3) for the case \( a = 1 \) we see that both exchange pulses of duration \( t \) shown in Fig. 2.4 multiply this state by a phase factor of \( e^{-it} \). Thus the \( ac = 1\frac{3}{2} \) diagonal element of the corresponding matrix representations is \( e^{-it} \).

Figure 2.5 shows a key three-pulse sequence used throughout our construction. The resulting unitary operation is denoted \( U_3 \). This pulse sequence is designed so that the matrix representation

\[
\begin{pmatrix}
e^{-it} \\
1 \\
\end{pmatrix}
\]

of\( U_3(\phi) \) introduces a phase difference \( \phi \) between the states \((\circ \circ)_1 \circ \circ)_{1/2} \) and \((\circ \circ)_1 \circ \circ)_{3/2} \). The graph of \( \phi \) vs. \( t \) shows that an arbitrary phase \( \phi \) can be generated by choosing \( t \) appropriately.

\[
\tan \frac{t}{2} \tan \frac{\tilde{t}}{2} = -2
\]

\[
\phi = t + \tilde{t} - \pi
\]

Figure 2.5: Sequence of three exchange pulses for \( U_3(\phi) \), a diagonal operation in the \((\circ \circ)_a \circ \circ)_{c} \) basis, shown for \( ac = \{0\frac{1}{2}, 1\frac{1}{2} 1\frac{3}{2}\} \). \( U_3(\phi) \) introduces a phase difference \( \phi \) between the states \((\circ \circ)_1 \circ \circ)_{1/2} \) and \((\circ \circ)_1 \circ \circ)_{3/2} \). The graph of \( \phi \) vs. \( t \) shows that an arbitrary phase \( \phi \) can be generated by choosing \( t \) appropriately.
Figure 2.6: Actions of the three rotations in the $c = 1/2$ pseudospin sector of the three-pulse sequence for $U_3$ shown in Fig. 2.5 on the vector $\hat{z}$. (a) The first pulse of duration $t$ rotates $\hat{z}$ about the $n_1$-axis to a vector on the yellow cone. (b) The second pulse of duration $\bar{t}$ rotates the resulting vector about the $z$-axis on the green cone. (c) Provided $\bar{t}$ is chosen (by solving (2.7)) so that after the first two rotations the resulting vector is on the intersection of the green and yellow cones, the third pulse of duration $t$ will rotate the vector about the $n_1$-axis back to $\hat{z}$. Because $\hat{z}$ is unchanged by this sequence, the resulting rotation is about the $z$-axis.

of $U_3$ is diagonal in the $((\bullet)_{a}\bullet)_{c}$ basis, as shown in Fig. 2.5 (up to an irrelevant overall phase factor, chosen so that the state $((\bullet)_{1}\bullet)_{1/2}$ is multiplied by 1). This allows us to treat the Hilbert space with $a = 0$ and $a = 1$ separately, while at the same time generating a phase difference of $\phi$ between the states $((\bullet)_{1}\bullet)_{1/2}$ and $((\bullet)_{1}\bullet)_{3/2}$. This phase difference is central to our construction and in what follows we will often write $U_3$ as a function of this phase, $U_3(\phi)$.

In the $c = 1/2$ sector, the pulse sequence for $U_3$ carries out three pseudospin rotations about first the $n_1$-, then $z$-, and again the $n_1$-axis through angles $t$, $\bar{t}$, and $t$, respectively. This sequence is chosen so that it results in a net rotation about the $z$-axis, and hence is diagonal in the $((\bullet)_{a}\bullet)_{1/2}$ basis. To find the relation between $t$ and $\bar{t}$ we determine the condition under which the vector $\hat{z}$ is unchanged under these three rotations. The yellow cone in Fig. 2.6(a) shows the set of vectors that $\hat{z}$ can be transformed into after rotations about the $n_1$-axis by the first pulse. For a particular choice of the first rotation angle $t$, the green cone in Fig. 2.6(b) then displays the set of possible outcomes of the second rotation, this time about the $z$-axis. The third rotation, again about the $n_1$-axis, must bring the transformed vector back to $\hat{z}$. Figure 2.6(c) shows both that there is only one non-zero choice for the second rotation angle, $\bar{t}$, and that the final rotation angle must again be $t$. It is a simple geometric exercise to show that the rotation angles $\bar{t}$ and $t$ are related by

$$\tan \frac{t}{2} \tan \frac{\bar{t}}{2} = \frac{1}{\hat{z} \cdot \hat{n}_1} = -2. \quad (2.7)$$
Furthermore, Fig. 2.6 clarifies that the $t, \bar{t}, t$ sequences are the only nontrivial sequences of three rotations that result in an effective $z$-axis rotation.

The sequence $t, \bar{t}, t$ produces the phase difference

$$\phi = t + \bar{t} - \pi$$

between the $((\bullet\bullet)_1\bullet)_{1/2}$ and $((\bullet\bullet)_1\bullet)_{3/2}$ states. As a function of the pulse length $t$, the phase $\phi$ varies monotonically from 0 to $2\pi$ (see Fig. 2.5). Thus, to produce $U_3(\phi)$ for a desired $\phi$ one need only solve for $t$ and $\bar{t}$ using (2.7) and (2.8). For a given $\phi$ there are two solutions, one with $0 \leq t < \pi \leq \bar{t} < 2\pi$, and another with $t \leftrightarrow \bar{t}$ so that $0 \leq \bar{t} < \pi \leq t < 2\pi$. The total duration of the $t, \bar{t}, t$ sequence with $t < \bar{t}$ is shorter than the sequence with $t > \bar{t}$, and we refer to the former as the short sequence and the latter as the long sequence. The only difference between the $U_3(\phi)$ operations produced by the short sequence and long sequence is the value of the phase factor $e^{-i\bar{t}}$ applied to the single state with $a = 0$, $((\bullet\bullet)_0\bullet)_{1/2}$. In our two-qubit gate construction we will see that the only effect the choice of this phase factor has is to determine the single-qubit rotations needed to bring the final gate to an exact controlled-phase gate form. We are thus free to use either the short or long sequence for each $U_3$ that appears in our construction (see Sec. 2.3.6).

### 2.3.3 Four Spins

In this section we turn to the four spins highlighted in Fig. 2.2(b) (labeled “Four Spins”), $((\bullet\bullet)_a(\bullet\bullet)_b)_d$ where $a$ and $b$ determine the states of the two logical qubits shown in Fig. 2.2(a).

The full Hilbert space of four spin-1/2 particles [as usual, not counting the $S_z$ degeneracy] is six-dimensional with one two-dimensional sector (total spin 0), one three-dimensional sector (total spin 1) and one one-dimensional sector (total spin 2). We reduce the nontrivial Hilbert space to that of a single spin-1/2 pseudospin by restricting ourselves to the use of the two operations shown in Fig. 2.7. One operation is the $U_3$ sequence described in Sec. 2.3.2 acting on the top three spins, the other is a simple exchange pulse $U_2$ between the bottom two spins.

Throughout our entire two-qubit gate construction (excluding single-qubit rotations), the top two spins with total spin labeled $a$, referring to Fig. 2.7, will only be acted on by $U_3$ operations.

---

3It is interesting to note that three pulse $t, \bar{t}, t$ sequences with $t$ and $\bar{t}$ satisfying (2.7) also appear in the 19-pulse sequence found numerically in Ref. [46]. Based on the geometric intuition provided by our construction it is possible to show that both short and long $t, \bar{t}, t$ sequences can be used in this 19-pulse sequence without changing the resulting two-qubit gate in the total spin-1 sector (up to single qubit rotations).
Because this operation is diagonal in the \([(\bullet\bullet)\bullet\bullet]_c\) basis, the value of \(a\) is conserved and we can treat the cases \(a = 0\) and \(a = 1\) separately. For the case \(a = 0\) the top three spins are always in the state \([(\bullet\bullet)\bullet\bullet]_{1/2}\). It follows that \(U_3\) acts as the identity times a phase factor on all states with \(a = 0\) in the full Hilbert space of the two encoded qubits. Provided we keep track of this \(a = 0\) phase (which will depend on whether we use the long or short sequence for \(U_3\)) as it accumulates we are free to focus on the case \(a = 1\) for which \(U_3\) acts nontrivially on a two-dimensional Hilbert space. At the end of our construction the \(a = 0\) phase factor can always be set to 1 by a single-qubit rotation acting on the left qubit in Fig. 2.2(a).

Since we need only consider the case \(a = 1\) in what follows we can represent the top two spins as a single spin-1 particle, as shown in Fig. 2.7. The basis states can then be written

\[
[(\bullet\bullet)_{a=1}\bullet\bullet]_d \rightarrow (\bigtriangleup\bullet\bullet)_b, \quad (2.9)
\]

where the symbol \(\bigtriangleup\) represents the effective spin-1 particle. This replacement of two spin-1/2 particles by one spin-1 particle is a key step in our construction.

The \(a = 1\) Hilbert space — spanned by a spin-1 and two spin-1/2 particles — is four-dimensional, with two one-dimensional sectors (total spin \(d = 0\) and 2) and one two-dimensional sector (total spin \(d = 1\)). The effective two-dimensional \(d = 1\) sector can be viewed in terms of a pseudospin where \(\uparrow = (\bigtriangleup\bullet\bullet)_{b=0}_1\) and \(\downarrow = (\bigtriangleup\bullet\bullet)_{b=1}_1\). As shown in Fig. 2.7, pulsing the exchange interaction between the bottom two spins for a time \(t\) then results in a \(z\)-axis rotation through angle \(t\) of this pseudospin.

The action of \(U_3\) on this two-dimensional Hilbert space is first seen most clearly in the \([(\bigtriangleup\bullet\bullet)\bullet\bullet]_{d=1}\) basis with \(c = \{1, 3/2\}\). Consulting Fig. 2.5 for the case \(a = 1\), we have

\[
U_{3,c}^{d=1} (t) = \begin{pmatrix} 1 & e^{-it} \\ e^{-it/2} & e^{it/2} \end{pmatrix} = e^{-it/2} e^{it\hat{n}_2 \cdot \sigma/2}. \quad (2.10)
\]

This operation acts like a nearest-neighbor exchange pulse between our effective spin-1 particle and its neighboring spin-1/2 particle. However, here the parameter \(t\) is not a pulse duration, but rather the value of the phase difference \(U_3(t)\) produces between the states \([(\bigtriangleup\bullet\bullet)_{1/2}\bullet\bullet]_1\) and \([(\bigtriangleup\bullet\bullet)_{3/2}\bullet\bullet]_1\), and is best viewed as an “effective” pulse time.

If we change back to the \((\bigtriangleup\bullet\bullet)_b)_{1}\) basis \(U_3\) becomes a pseudospin rotation about an axis \(\hat{n}_2\). To determine \(\hat{n}_2\) we again need to carry out a basis change using the relevant recoupling coefficients,
Figure 2.7: Two operations, a simple exchange pulse $[U_2(t)]$ and $U_3(t)$, acting on the Hilbert space of four spins. Both operations conserve $a$ and act trivially on states with $a = 0$. This allows us to focus on the case $a = 1$ by replacing the two spins with total spin $a$ by an effective spin-1 particle represented by $\blacktriangle$. The matrix representations of $U_2(t)$ and $U_3(t)$ are then given in the $bd = \{10|01,11|12\}$ basis. In the $d = 1$ sector, $U_2(t)$ and $U_3(t)$ carry out rotations about $\hat{z}$ and $\hat{n}_2 = (-2\sqrt{2}/3, 0, -1/3)$, respectively, for a pseudospin where $\uparrow = (\blacktriangle\bullet\bullet)_0$ and $\downarrow = (\blacktriangle\bullet\bullet)_1$.

this time for one spin-1 particle and two spin-1/2 particles with total spin 1,

$$(\blacktriangle\bullet\bullet)_b = \sum_c F_{2, bc}((\blacktriangle\bullet\bullet)_c)_1, \quad (2.11)$$

where $F_{2, bc} = \langle((\blacktriangle\bullet\bullet)_c)_1|((\blacktriangle\bullet\bullet)_b)_1\rangle$. The matrix

$$F_2 = \begin{pmatrix} -1/\sqrt{3} & \sqrt{2/3} \\ \sqrt{2/3} & 1/\sqrt{3} \end{pmatrix} = \hat{f}_2 \cdot \sigma \quad (2.12)$$

then changes bases from $((\blacktriangle\bullet\bullet)_c)_1$ with $c = \{1/2, 3/2\}$ to $(\blacktriangle\bullet\bullet)_b$ with $b = \{0,1\}$, where $\hat{f}_2 = (\sqrt{2/3}, 0, -1/\sqrt{3})$. The action of $U_3(t)$ on the $d = 1$ sector in the original basis is then

$$U_{3,b}^{d=1}(t) = F_2 U_{3,c}^{d=1}(t) F_2 = e^{-it/2} e^{it\hat{n}_2 \cdot \sigma/2}, \quad (2.13)$$

where the rotation axis $\hat{n}_2 = 2\hat{f}_2(\hat{f}_2 \cdot \hat{z}) - \hat{z} = (-2\sqrt{2}/3, 0, -1/3)$ makes an angle $\cos^{-1} \hat{n}_2 \cdot \hat{z} = \cos^{-1} -1/3$ with the $z$-axis, as shown in Fig. 2.7.
Figure 2.8: Sequence of exchange pulses ($U_2$) and $U_3$ operations acting on four spins resulting in the operation $U_4(\phi)$. The sequence is constructed so that the matrix representation of $U_4(\phi)$ is diagonal in the $(\bigtriangleup \bigcirc \bigstar)_b d$ basis, shown for $bd = \{10|01\}, 11|12\}$. The two-step similarity transformation that diagonalizes the $d = 1$ block of $U_3(\phi)$ in this basis is illustrated by the two intersecting cones where $t_4 = 2\pi/3$ and, for the inverse operation, $s_4 = 2\pi - t_4 = 4\pi/3$.

Finally, note that for the sectors with total spin $d = 0$ and 2 the change of bases is trivial: $(\bigtriangleup \bigcirc \bigstar)_b d = 0 = \left((\bigtriangleup \bigcirc \bigstar)_c = 1/2 \bigstar\right)_0$ and $(\bigtriangleup \bigcirc \bigstar)_b d = 2 = \left((\bigtriangleup \bigcirc \bigstar)_c = 3/2 \bigstar\right)_2$. Consulting Fig. 2.5, we see that $U_3(t)$ multiplies the states with $d = 0$ and $d = 2$ by 1 and $e^{-it}$, respectively, while from (2.1) the exchange pulse $U_2(t)$ acting on the bottom two spins multiplies both states by $e^{-it}$. The resulting full matrix representations of $U_2(t)$ and $U_3(t)$ are given in Fig. 2.7.

At the next level of our construction we will need an operation which is diagonal in the $(\bigtriangleup \bigcirc \bigstar)_b d$ basis. This will allow us to treat the Hilbert space with $b = 0$ and $b = 1$ separately. The simplest way to produce such a diagonal operation would be to pulse the exchange interaction between the bottom two spins with total spin $b$ (see Fig. 2.7). However, such a pulse will merely correspond to a single-qubit rotation, and therefore is not useful for our two-qubit gate construction.

Given that three operations are not sufficient we turn to sequences with five operations (sequences with four operations are equivalent to sequences with three operations up to a single-qubit rotation). Figure 2.8 shows such a sequence that produces a diagonal operation which will be useful at the next level of our construction. The sequence has the form $U_4(\phi) = U_3(s_4)U_2(t_4)U_3(\phi)U_2(s_4)U_3(s_4)$, where $s_4 = 2\pi - t_4$ so that $U_2(s_4) = U_2(t_4)^{-1}$ and $U_3(s_4) = U_3(t_4)^{-1}$.
in the $a = 1$ Hilbert space. Thus, in this space, $U_4(\phi) = SU_3(\phi)S^{-1}$ where $S = U_3(t_4)U_2(t_4)$. Written in this way, it is clear that $U_4(\phi)$ is the result of carrying out a similarity transformation on the $U_3(\phi)$ operation at the center of the sequence. In the two-dimensional $d = 1$ sector this transformation can be understood geometrically as a rotation generated by $U_3(t_4)U_2(t_4)$, two pseudospin rotations about first the $z$-axis and then the $n_2$-axis, both through angle $t_4$. These rotations act on $\hat{n}_2$, the rotation axis of $U_3(\phi)$, and are designed to diagonalize $U_3(\phi)$ in the $(\boldsymbol{\bigtriangleup}\boldsymbol{\bullet\bullet})_b$ basis by rotating $\hat{n}_2$ to $\hat{z}$.

The transformation of the rotation axis of $U_3(\phi)$ from $\hat{n}_2$ to $\hat{z}$ is illustrated in Fig. 2.8. Rotating $\hat{n}_2$ (\hat{z}) about the $z$-axis ($n_2$-axis) results in the rotated vector lying somewhere on the green (yellow) cone. The rotation angle $t_4$ is chosen so that $\hat{n}_2$ is first rotated about the $z$-axis to where the two cones intersect. This is then followed by a rotation about the $n_2$-axis through the same angle so that the final rotated vector is $\hat{z}$. It is straightforward to calculate the required rotation angle,

$$t_4 = \cos^{-1} \left( \frac{\hat{n}_2 \cdot \hat{z}}{\hat{n}_2 \cdot \hat{z} + 1} \right) = \frac{2\pi}{3}. \quad (2.14)$$

Due to this similarity transformation $U_4(\phi) = SU_3(\phi)S^{-1}$, the matrix representation of $U_4(\phi)$ in the $d = 1$ sector in the $(\boldsymbol{\bigtriangleup}\boldsymbol{\bullet\bullet})_b$ basis with $b = \{0, 1\}$ is a $z$-axis rotation,

$$U_{4,b}^{d=1}(\phi) = e^{-i\phi/2}e^{i\phi/2} = \begin{pmatrix} 1 \\ e^{-i\phi} \end{pmatrix}. \quad (2.15)$$

The full matrix representation of $U_4(\phi)$ in all sectors is shown in Fig. 2.8. Since in the one-dimensional sectors with $bd = 10$ and $bd = 12$ the similarity transformation $U_4(\phi) = SU_3(\phi)S^{-1}$ has no effect on $U_3(\phi)$, the corresponding elements are 1 and $e^{-i\phi}$, respectively (see Fig. 2.7).

Let us summarize what we have achieved at this point and what still needs to be done to construct an entangling two-qubit gate. The operation $U_4(\phi)$ multiplies the only $ab = 10$ state, $(\boldsymbol{\bigtriangleup}\boldsymbol{\bullet\bullet})_{b=0,d=1}$, by 1 while multiplying two of the three $ab = 11$ states, $(\boldsymbol{\bigtriangleup}\boldsymbol{\bullet\bullet})_{d=1,2}$, by the phase factor $e^{-i\phi}$. If this operation also multiplied $(\boldsymbol{\bigtriangleup}\boldsymbol{\bullet\bullet})_{d=0}$ by the same phase factor, the action of $U_4(\phi)$ would be to apply a controlled-phase gate (up to the single-qubit rotation needed to eliminate the $a = 0$ phase discussed above) on the two encoded qubits in Fig. 2.2(a) in which the state $ab = 11$ acquires a phase factor $e^{-i\phi}$ while the states $ab = 00, 01, 10$ are multiplied by 1. However, this is not the case because $U_4(\phi)$ multiplies $(\boldsymbol{\bigtriangleup}\boldsymbol{\bullet\bullet})_{d=0}$ by 1. This is consistent with the result of the theorem proved in Sec. 2.3.7 which shows that any sequence of exchange pulses acting on only four
spins cannot result in a leakage-free entangling two-qubit gate. To achieve such a gate, we need to consider pulse sequences which act on one more spin.

2.3.4 Five Spins

We now turn to the final stage of our controlled-phase gate construction which involves five spins. These spins are highlighted in Fig. 2.2(b) (labeled “Five Spins”) in the \((\bullet\bullet)_{a}(\bullet\bullet)_{b}\) basis with \(a\) and \(b\) determining the state of the two encoded qubits shown in Fig. 2.2(a).

The full Hilbert space of five spin-1/2 particles is ten-dimensional and breaks into a five-dimensional sector (total spin 1/2), a four-dimensional sector (total spin 3/2), and a one-dimensional sector (total spin 5/2). With reference to Fig. 2.2, note that because the total spin of all six spin-1/2 particles encoding two logical qubits can only be either \(g = 0\) or \(g = 1\), the one-dimensional \(f = 5/2\) sector is not relevant for our two-qubit gate construction.

We use the two operations \(U_3(t)\) and \(U_4(t)\) shown in Fig. 2.9 to construct the controlled-phase gate, where \(U_3\) now acts on the bottom three spins and \(U_4\) on the top four spins. In addition to conserving
a, for the reasons given in Sec. 2.3.3, these operations also conserve b. For the case b = 0 the top four spins are always in the state \((\bigtriangleup (\bullet \bullet)_{0})_{1}\) and the bottom three spins are always in the state \(((\bullet \bullet)_{0} \bullet)_{1/2}\). From Fig. 2.8 we then see that \(U_4\) acts as the identity and, from the discussion in Sec. 2.3.3, \(U_3\) acts as the identity times a phase factor (which depends on whether we use the short or long sequence) on all states with \(b = 0\) in the full Hilbert space of the two encoded qubits. As for the \(a = 0\) phase factor discussed in Sec. 2.3.3, if we keep track of this \(b = 0\) phase factor we are free to focus entirely on the case \(b = 1\). The \(b = 0\) phase factor can then be set to 1 by a single-qubit rotation acting on the qubit on the right in Fig. 2.2(a). The only nontrivial case is thus \(ab = 11\).

To construct a controlled-phase gate we need to multiply this state with a phase factor of \(e^{-i\phi}\). We exploit the fact that \(ab = 11\) is the only nontrivial case by working in the reduced Hilbert space of five spin-1/2 particles in which the two spins labeled \(a\) and the two spins labeled \(b\) are both replaced by effective spin-1 particles, as also shown in Fig. 2.9. The effective Hilbert space is then that of one spin-1/2 and two spin-1 particles and has two two-dimensional sectors for \(f = 1/2\) and 3/2 (again, as shown above, we need not consider the \(f = 5/2\) sector). In both sectors we define a pseudospin \(\uparrow_f = (\bigtriangleup (\bullet \bullet)_{e=1/2})_f\) and \(\downarrow_f = (\bigtriangleup (\bullet \bullet)_{e=3/2})_f\).

The matrix representations of \(U_3\) and \(U_4\) in the \((\bigtriangleup (\bullet \bullet)_{e})_f\) basis are shown in Fig. 2.9. Referring to Fig. 2.5 for the case \(a = 1\), we see that in this basis \(U_3\) performs a pseudospin rotation about the \(z\)-axis in both the \(f = 1/2\) and 3/2 sectors. The action of \(U_4\) is most easily seen in the \(((\bigtriangleup \bullet)_{d})_f\) basis where, from Fig. 2.8 for the case \(b = 1\), we know the matrix representation in the \(f = 1/2\) sector and the \(df = \{0 \frac{1}{2}, 1 \frac{1}{2}\}\) basis is

\[
U_{4,df}^{f=1/2}(t) = \begin{pmatrix} 1 & e^{-it} \\ e^{-it/2} e^{it/2} & 1 \end{pmatrix} = e^{-it/2} e^{it/2} \sigma_z/2;
\]

and in the \(f = 3/2\) sector and the \(df = \{1 \frac{3}{2}, 2 \frac{3}{2}\}\) basis is

\[
U_{4,df}^{f=3/2}(t) = \begin{pmatrix} e^{-it} & 0 \\ 0 & e^{it} \end{pmatrix} = e^{it} \mathbb{1}.
\]

To determine the action of \(U_4\) on the \(f = 1/2\) sector in the \((\bigtriangleup (\bullet \bullet)_{e})_f\) basis we once again perform a basis change,

\[
((\bigtriangleup (\bullet \bullet)_{e})_{1/2}) = \sum_{d} F_{3,ed} ((\bigtriangleup \bullet)_{d})_{1/2},
\]

as also shown in Fig. 2.9. The effective Hilbert space is then that of one spin-1/2 and two spin-1 particles and has two two-dimensional sectors for \(f = 1/2\) and 3/2 (again, as shown above, we need not consider the \(f = 5/2\) sector). In both sectors we define a pseudospin \(\uparrow_f = (\bigtriangleup (\bullet \bullet)_{e=1/2})_f\) and \(\downarrow_f = (\bigtriangleup (\bullet \bullet)_{e=3/2})_f\).
Figure 2.10: (a) Sequence of operations $U_3$ and $U_4$ acting on five spins resulting in the operation $U_5(\phi)$. The sequence is constructed so that the matrix representation of $U_5(\phi)$ is diagonal in the $(\dagger\dagger\dagger\dagger\dagger)_{ef}$ basis, shown for $ef = \{\frac{1}{2}, \frac{3}{2}\}$. The two-step similarity transformation which carries out this diagonalization is illustrated by the two intersecting cones, where $t_5 = \cos^{-1}(1/4)$ and $s_5 = 2\pi - t_5$. (b) Controlled-phase gate consisting of $U_5(\phi)$ acting on five spins of two encoded qubits together with two exchange pulses of times $t_a$ and $t_b$ that carry out two single-qubit rotations which depend on the particular choice of short or long $U_3$ sequences.

where $F_{3,ed} = \langle ((\dagger\dagger\dagger\dagger\dagger)_{d})_{1/2}|(\dagger\dagger\dagger\dagger\dagger)_{e}_{1/2} \rangle$. The corresponding $2 \times 2$ matrix is the same as $F_2$ (a fact which can be understood using the symmetries of the Wigner $6j$ symbol, see, e.g., Ref. [117]), and generates a basis change from the $d = \{0, 1\}$ basis to the $e = \{\frac{1}{2}, \frac{3}{2}\}$ basis,

$$F_3 = \begin{pmatrix} \frac{-1}{\sqrt{3}} & \frac{\sqrt{2}}{3} \\ \frac{\sqrt{2}}{3} & \frac{1}{\sqrt{3}} \end{pmatrix} = \hat{f}_2 \cdot \sigma. \quad (2.20)$$

It follows that

$$U_{4,e}^{f=1/2}(t) = F_3 U_{4,d}^{f=1/2}(t) F_3 = e^{-it/2} e^{it\hat{n}_2 \cdot \sigma/2}, \quad (2.21)$$

where $\hat{n}_2$ is the same rotation axis found in Sec. 2.3.3. Since in the $f = 3/2$ sector $U_4$ is proportional to the identity it will be left unchanged by the basis change to the $(\dagger\dagger\dagger\dagger\dagger)_{e}_{3/2}$ basis,

$$U_{4,e}^{f=3/2}(t) = U_{4,d}^{f=3/2}(t) = e^{-it}\mathbb{1}. \quad (2.22)$$

At this point we are ready to complete our two-qubit gate construction. To do this, we need to produce a sequence of operations acting on five out of the six spins forming the two encoded qubits in states $a$ and $b$ (see Fig. 2.2(a)) which applies a phase factor of $e^{-i\phi}$ to the state with $ab = 11$. To
see what is required note that the two-qubit state $|1_L\rangle|1_L\rangle$ can be expressed as $((\bullet\Box)_{1/2}(\bullet\Box)_{1/2})_g$ where $g$ equals 0 or 1. It is straightforward to expand these states as follows,

$$((\bullet\Box)_{1/2}(\bullet\Box)_{1/2})_0 = ((\bullet\Box)_{1/2}(\bullet\Box)_{1/2})_{f=1/2}$$  \hspace{1cm} (2.23)

$$((\bullet\Box)_{1/2}(\bullet\Box)_{1/2})_1 = -\frac{1}{3}((\bullet\Box)_{1/2}(\bullet\Box)_{1/2})_{f=1/2} + \frac{2\sqrt{2}}{3}((\bullet\Box)_{1/2}(\bullet\Box)_{1/2})_{f=3/2}$$  \hspace{1cm} (2.24)

where in (2.24) we have used the recoupling coefficients $F_{4,1/2} = ((\bullet\Box)_{1/2}((\bullet\Box)_{1/2}^1)_{1}((\bullet\Box)_{1/2}^1)_{1})$ where $F_{4,1/2} = -1/3, F_{4,3/2} = 2\sqrt{2}/3$. Here the rightmost $\bullet$ in the definition of $F_4$ represents the rightmost qubit in the state $(\bullet\Box)_{1/2}$ in (2.24). To apply a phase factor of $e^{-i\phi}$ to both states on the left-hand sides of (2.23) and (2.24) it is clearly necessary to apply this same phase factor to the five-spin states $(\bullet\Box)_{1/2}$ and $(\bullet\Box)_{1/2}$3/2. We therefore need to find a sequence of operations that produces an operation diagonal in the $(\bullet\Box)_{1/2}$ basis.

The simplest such diagonal operation is produced by a single action of the operation $U_3$. However, as can be seen in Fig. 2.9, this operation applies a different phase factor to the states $(\bullet\Box)_{1/2}$f=1/2 and $(\bullet\Box)_{1/2}$f=3/2. It is then natural to again try to apply the three-operation construction $U_4(t)U_3(t)U_4(t)$ of Sec. 2.3.2. However, as in Sec. 2.3.3, this construction is incapable of producing the required operation. Direct calculation shows that it is impossible to produce an operation for which the same nontrivial phase factor is applied to the states $(\bullet\Box)_{1/2}$f with $f = 1/2$ and $f = 3/2$. Performing four operations, i.e. a sequence of the form $U_3U_4U_3U_4$, is equivalent to $U_4U_3U_4$ because the final $U_3$ operation is a single-qubit rotation. We must therefore consider a sequence of at least five operations, and the explicit construction presented below shows that five is indeed enough.

The sequence shown in Fig. 2.10(a) is designed to multiply the two states $(\bullet\Box)_{1/2}$f=1/2,3/2 by the same phase factor of $e^{-i\phi}$. The sequence has the form $U_5(\phi) = U_4(s_5)U_3(t_5)U_4(\phi)U_5(s_5)U_4(t_5)$ where $s_5 = 2\pi - t_5$ so that $U_4(s_5) = U_4(t_5)^{-1}$ and $U_3(s_5) = U_3(t_5)^{-1}$ in the $ab = 11$ Hilbert space. Similar to $U_4$ in Sec. 2.3.3, in this space the $U_5$ construction has the structure of a similarity transformation, $U_5(\phi) = S(U_4(\phi)S^{-1}$ with $S = U_4(s_5)U_3(t_5)$. In both the $f = 1/2$ and $f = 3/2$ sectors this similarity transformation can be visualized as a series of pseudospin rotations.

Again referring to Fig. 2.9 for the case of $f = 3/2$, $U_4(\phi)$ is equal to the identity times $e^{-i\phi}$. This immediately implies that in this sector the similarity transformation has no effect. Thus, in the $f = 3/2$ sector, $U_5(\phi)$ equals $U_4(\phi)$ and, in particular, multiplies the state $(\bullet\Box)_{1/2}$3/2 by $e^{-i\phi}$. 

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To understand the action of $U_5(\phi)$ on the $f = 1/2$ sector, note that in this sector $U_4(\phi)$ is a pseudospin rotation about the axis $\hat{n}_2$. In order for $U_5(\phi)$ to multiply the state $(\uparrow(\uparrow\bullet)_{1/2})_{1/2}$ by $e^{-i\phi}$, the similarity transformation carried out by $S$ in this sector must be chosen so that it rotates $\hat{n}_2$, the rotation axis of $U_4(\phi)$, to $-\hat{z}$. As shown in Fig. 2.10, $S$ consists of a rotation about the $z$-axis through the angle $t_5$ (green cone) followed by a rotation about the $n_2$-axis through the angle $s_5 = 2\pi - t_5$ (yellow cone). It is straightforward to show that if we choose $t_5 = \cos^{-1} \frac{\hat{n}_2 \cdot \hat{z}}{\hat{n}_2 \cdot \hat{z} - 1}$, then, under these rotations, $\hat{n}_2$ is first rotated to the intersection of the green and yellow cones, and then rotated to $-\hat{z}$.

The outcome of this transformation in the $f = 1/2$ sector of $U_5(\phi)$ in the $(\uparrow(\uparrow\bullet)e)_{1/2}$ basis with $e = \{\frac{1}{2}, \frac{3}{2}\}$ is

$$U_{5,e}^{f=1/2}(\phi) = e^{-i\phi/2} e^{i\phi(-\hat{z})\cdot\sigma/2} = \begin{pmatrix} e^{-i\phi} & 0 \\ 0 & 1 \end{pmatrix}. \quad (2.26)$$

Thus the state with $((\bullet\bullet)_{a=1}(\bullet\bullet)_{b=1\bullet})_{1/2}$ is multiplied by a phase factor of $e^{-i\phi}$. As shown above, in the $f = 3/2$ sector $U_5(\phi)$ is proportional to the identity and multiplies the state $((\bullet\bullet)_{a=1}(\bullet\bullet)_{b=1\bullet})_{3/2}$ by the same phase factor of $e^{-i\phi}$. So the action of $U_5(\phi)$ is to multiply all states with $g = 0$ and 1 on the right-hand sides of (2.23) and (2.24) by $e^{-i\phi}$.

The resulting operation is thus locally equivalent to a controlled-phase gate. To complete the gate construction we need only determine the single-qubit rotations needed to set the $a = 0$ phase factor, discussed in Sec. 2.3.3, and the $b = 0$ phase factor, discussed above, to 1. The value of these phase factors depend on whether we use short sequences or long sequences for the $U_3$ operations throughout the construction. Whatever the value of these phase factors, they can be set to 1 by performing single-qubit rotations corresponding to the two pulses shown in Fig. 2.10(b).

### 2.3.5 Comment on Sequences Acting on at most Five Spins

Consider the two qubits in states $a$ and $b$ shown in Fig. 2.2(a) whose state is given by

$$((\bullet\bullet)_{a=1}(\bullet\bullet)_{b=1\bullet})_{g=0, 1}. \quad (2.27)$$

In Sec. 2.1 we pointed out that the pulse sequence found by DiVincenzo et al. in Ref. [46] carries out an entangling two-qubit gate only in the total-spin $g = 1$ sector but not in the $g = 0$ sector. In
contrast, the family of pulse sequences established above, as well as the Fong-Wandzura sequence [101], carry out the same two-qubit gate in both $g$ sectors. As we discuss now, this discrepancy is no unrelated to the number of spins that the respective sequences are acting on.

Indeed, we remark that any sequence of exchange pulses that acts on only five spins and that carries out a leakage-free two-qubit gate in the total-spin $g = 1$ sector, will automatically carry out the very same gate in the total-spin $g = 0$ sector. To show this, we assume without loss of generality that the sequence acts onto the five rightmost spins whose Hilbert space basis we take to be

$$(((\bullet)(\bullet))_{g=\frac{1}{2}}).$$

(2.28)

Note that i) any such sequence acting on only the five rightmost spins conserves $f$; and ii) for both $g = 0$ and $g = 1$ the two-qubit basis states in Eq. (2.27) with $ab = 00, 01, 10, \text{ and } 11$ all have nonzero projection onto the $f = 1/2$ sector. [For $g = 0$, $f$ is fixed to be $1/2$. For $g = 1$, when $a = 0$, $f$ is also fixed to be $1/2$, and, when $a = 1$, the expansion (2.24), together with a similar expansion for the case $b = 0$ with the same recoupling coefficients, implies nonzero projection onto the $f = 1/2$ sector.] Any operation produced by a pulse sequence which acts on the five rightmost spins will then have identical matrix representations in two two-qubit subspaces with the same $ab$ basis choice: one in the $g = 0$ sector, which lives entirely in the $f = 1/2$ sector, and another in the $g = 1$ sector, after projection onto the $f = 1/2$ sector. Therefore, if this sequence produces a leakage-free two-qubit gate in the $g = 1$ sector it will produce the same leakage-free two-qubit gate in $g = 0$ sector.

This observation is consistent with the fact that the Fong-Wandzura sequence[101] and related sequences in Ref. [114], as well as our sequences, act on only five spins, while the sequence of Ref. [46] acts on six.

2.3.6 Full Pulse Sequences

Figure 2.11 shows two explicit pulse sequences for controlled-phase gates obtained by unpacking the $U_4$ and $U_3$ operations in Fig. 2.10 and replacing them with sequences of exchange pulses. To do this unpacking, each $U_3$ operation, including those within each $U_4$ operation, are replaced by three-pulse sequences found by solving (2.7) and (2.8) (see Sec. 2.3.2). To determine the pulse times for the entire sequence it is necessary to solve these equations for $U_3(x)$ where $x = t_4, t_5, s_4, s_5$ (see
Figure 2.11: Two full pulse sequences of 39 pulses plus single qubit rotations for the controlled-phase gate construction shown in Fig. 2.10(b): (a) a 40-pulse sequence (with one single-qubit rotation); and (b) a 41-pulse sequence (with two single-qubit rotations) of slightly shorter total duration obtained by swapping pulse labels $s_1 \leftrightarrow \bar{s}_1$ and $s_2 \leftrightarrow \bar{s}_2$.

Red pulses depend on the phase $\phi$ which determines the controlled-phase gate, and black pulses are independent of $\phi$. Ignoring single-qubit rotations, the pulse times which do not depend on $\phi$ are $t_4 = 2\pi/3$, $s_4 = 4\pi/3$, as well as $t_1 = 1.34004$ and $t_2 = 0.86463$ (obtained by solving for the short sequences for $U_3(t_4)$ and $U_3(t_5 = \cos^{-1}(1/4))$, respectively, see Sec. 2.3.2), together with those obtained from the relations $\tan(t_i/2)\tan(\bar{t}_i/2) = -2$ and $t_i + \bar{s}_i = t_i + s_i = 2\pi$ for $i = 1, 2$. The times $t$ and $\bar{t}$ depend on $\phi$ and are found by solving for the short or long sequence for $U_3(\phi)$. In (a) a single pulse of duration $\bar{t}$ brings the final gate to controlled-phase gate form, whereas in (b) two pulses acting on both qubits are required, with pulse durations $t_a = 4.11499 + \bar{t}$ (mod $2\pi$) and $t_b = 2.73045$. For $\phi = \pi$ the controlled-phase gate carried out by these pulse sequences is locally equivalent to CNOT and, if we choose the short sequence for the central $U_3(\phi = \pi)$, we find $t = 1.91063$ and $\bar{t} = 4.37255$.

Secs. 2.3.3 and 2.3.4), as well as $x = \phi$ where $\phi$ is the phase which characterizes the controlled-phase gate. The two sequences shown in Fig. 2.11 correspond to different choices for the two possible three-pulse sequences that can be used to carry out each $U_3$ operation, the short sequence and the long sequence.

In Fig. 2.11(a) each $U_3(t_4)$ and $U_3(t_5)$ are taken to be short sequences, while each $U_3(s_4)$ and
$U_3(s_5)$ are taken to be long sequences. For this choice $U_3(s_4) = U_3(t_4)^{-1}$ and $U_3(s_5) = U_3(t_5)^{-1}$ in the full Hilbert space, not just in the $ab = 11$ subspace. As a consequence, from the palindromic form of the full sequence, it is apparent that the $a = 0$ phase factors contributed by those $U_3$ operations which act on the two spins in the state $a$ cancel, save that due to the single $U_3(\phi)$ in the center of the sequence for $U_4(\phi)$, which is itself at the center of the sequence for $U_5(\phi)$. This phase factor is eliminated by the single-qubit rotation carried out by the single red pulse at the end of the sequence. The $b = 0$ phase factors contributed by $U_3(s_5)$ and $U_3(t_5)$ in Fig. 2.10(a) cancel completely and there is no need for a single-qubit rotation on the qubit in the state $b$. All of the pulse times are fixed except for the four pulses shown in red: three in the center, with times labeled $t$, $\bar{t}$, and $t$, which carry out $U_3(\phi)$, and the one at the end of the sequence mentioned above of time $\bar{t}$ which removes the $a = 0$ phase factor. The pulse times, including those for the $\phi$-dependent red pulses when $\phi = \pi$, are given explicitly in the figure caption.

In Fig. 2.11(b) we continue to take each $U_3(t_4)$ and $U_3(t_5)$ to be short sequences, but now also take each $U_3(s_4)$ and $U_3(s_5)$ to be short sequences. The resulting full sequence then has slightly shorter total duration than that shown in Fig. 2.11(a) provided all pulses are performed in parallel when possible. Switching to only short sequences amounts to swapping the pulses of length $s_i$ with those of length $\bar{s}_i$ for $i = 1$ and 2 in Fig. 2.11(a). The price of this rearrangement is that we lose the phase factor cancellations which occurred in the first sequence. Because of this, two single-qubit rotations corresponding to the two pulses at the end of the sequence, rather than just one, are needed to eliminate the $a = 0$ and $b = 0$ phase factors. One pulse acts on the two spins in the state $a$ for time $t_a$ which depends on $\phi$ through $\bar{t}$, and the second pulse acts on the two spins in the state $b$ for time $t_b$ which is independent of $\phi$. Both $t_a$ (as a function of $\bar{t}$) and $t_b$ are given in the figure caption.

The 39-pulse sequences given in this section here are significantly longer than other known sequences that can be used to carry out entangling two-qubit gates. As we see in Sec. 2.4, using the same operations $U_3$ and $U_4$ derived in Secs. 2.3.2 and 2.3.3 one can construct a two-qubit gate sequence that is similar to the one shown here, but which consists of only 25 pulses.

### 2.3.7 Four Spins are Not Enough

Here we show that any sequence of exchange pulses which carries out a leakage-free, entangling two-qubit gate on two three-spin qubits, independent of whether the total spin of all six particles
is 0 or 1, must act on at least five spins.\footnote{This proof is closely related to that given in Ref. [116] showing that for so-called SU(2)_k anyons for k > 3 it is necessary to braid at least five anyons to carry out similar two-qubit gates on qubits encoded using three anyons, and can be viewed as the k → ∞ limit of this proof.}

To do this it is convenient to consider logical qubits encoded using four spins rather than just three. This four-spin encoding is shown in Fig. 2.12(a) (the noncomputational states are those for which the total spin of the four spin-1/2 particles is 1 or 2). Figure 2.12(b) shows two adjacent four-spin qubits, and illustrates the fact that if we remove the two outermost spins the remaining three spins in each logical qubit have total spin 1/2 and are therefore precisely the three-spin qubits used in our main construction. Thus any pulse sequence which performs a two-qubit gate on two three-spin qubits regardless of whether their total spin is 0 or 1 must carry out the same two-qubit gate on two four-spin qubits when acting on the six central spins in Fig. 2.12(b).

It follows that the Fong-Wandzura sequence, as well as our sequences, can be used to carry out two-qubit gates on pairs of four-spin qubits. We note that a 34-pulse sequence which produces a two-qubit gate locally equivalent to CNOT for two four-spin qubits was also found numerically in Ref. [111] using methods similar to those used in Ref. [46]. However, this sequence acts on all eight spins used to encode the two qubits and thus cannot be used to carry out two-qubit gates for three-spin qubits.

Now consider an operation produced by exchange pulses which only act on the four central spins, i.e. those circled by the dashed line labeled by the total enclosed spin d, in Fig. 2.12(c).
We denote the resulting unitary operation $U^{(4)}$. If we assume that $U^{(4)}$ carries out a leakage-free two-qubit gate then it is clear that $U^{(4)}$ must be diagonal in the $((\bullet \bullet)_a (\bullet \bullet)_b)_d$ basis. If this were not the case then either $a$, $b$, or both would change after carrying out $U^{(4)}$. As a result, one or both of the four-spin qubits would undergo a transition to a state in which the two pairs of spins within the qubit have different total spin values. Since any such four-spin state cannot have total spin 0, this transition would lead to leakage out of the encoded four-spin qubit space shown in Fig. 2.12(a).

Since $U^{(4)}$ is diagonal in the $((\bullet \bullet)_a (\bullet \bullet)_b)_d$ basis it must give each encoded two-qubit state in the $a b$ basis a phase factor, $e^{i\phi_{ab}}$. For the two-qubit states with $a b = 00, 01, 10$ the value of the total spin $d$ is fixed to be 0, 1, and 1, respectively, and so the corresponding phase factors are single elements in the matrix representation of $U^{(4)}$. However, for the case $a b = 11$ the value of $d$ can be either 0, 1 or 2. Moreover, states with all three $d$ values have non-zero overlap with two four-spin qubits in the $a b = 11$ state. To see this, first express this state, $((\bullet \bullet)_a=1(\bullet \bullet)_a=1)((\bullet \bullet)_b=1(\bullet \bullet)_b=1)_0$, as $(\uparrow \uparrow)_0(\uparrow \uparrow)_0$ (where, as in the main text, $\uparrow$ is an effective spin-1 particle). This state can then be expanded in basis states with well-defined $d$ quantum numbers as follows,

$$((\uparrow \uparrow)_0(\downarrow \downarrow)_0)_0 = (\uparrow(\uparrow \downarrow)_0)_0$$
$$= \frac{1}{3}(\uparrow((\downarrow \downarrow)_{d=0}\uparrow)_1)_0 - \frac{1}{\sqrt{3}}(\uparrow((\downarrow \downarrow)_{d=1}\uparrow)_1)_0 + \frac{\sqrt{5}}{3}(\uparrow((\downarrow \downarrow)_{d=2}\uparrow)_1)_0,$$

where we have used the recoupling coefficients $F_{5,0d} = \langle((\downarrow \downarrow)_{d}\uparrow)|((\downarrow \downarrow)_{0}\uparrow)_1\rangle$ where $F_{5,00} = 1/3$, $F_{5,01} = -1/\sqrt{3}$, and $F_{5,02} = \sqrt{5}/3$. Since these coefficients are non-zero for all possible values of $d$, the phase factor, $e^{i\phi_{11}}$, produced by $U^{(4)}$ for the state $a b = 11$ must be the same for $d$ = 0, 1, and 2.

The above discussion shows that in the $((\bullet \bullet)_a (\bullet \bullet)_b)_d$ basis with $a b d = \{000, 110|011, 101, 111|112\}$, the matrix representation of $U^{(4)}$ must have the form

$$U^{(4)} = \begin{pmatrix} e^{i\phi_{00}} & e^{i\phi_{11}} \\ e^{i\phi_{01}} & e^{i\phi_{10}} \end{pmatrix}.$$

It is straightforward to show that the two-qubit gate produced by $U^{(4)}$ is locally equivalent to a controlled rotation through the angle $\phi = \phi_{00} - \phi_{01} + \phi_{10} + \phi_{11}$. The requirement that $U^{(4)}$ produce
an entangling two-qubit gate is then

$$\phi_{00} - \phi_{01} - \phi_{10} + \phi_{11} \neq 0 \quad \text{(mod } 2\pi).$$  \tag{2.31}$$

We denote the determinant of \( U^{(4)} \) in a sub-sector of total spin \( d \) as \( \det U^{(4)}|_{d} \). Equations (2.30) and (2.31) then imply the following condition on \( U^{(4)} \),

$$\frac{\det U^{(4)}|_{d=0} \det U^{(4)}|_{d=2}}{\det U^{(4)}|_{d=1}} \neq 1. \tag{2.32}$$

If \( U^{(4)} \) is the result of a series of \( N \) exchange pulses it has the form

$$U^{(4)} = U_N(t_N) \cdots U_2(t_2)U_1(t_1). \tag{2.33}$$

Here \( U_n(t_n) = \exp(-i\mathcal{H}_n t_n) \) is the time evolution operator of the \( n \)-th pulse, where \( \mathcal{H}_n = \mathbf{S}_{i(n)} \cdot \mathbf{S}_{j(n)} + \frac{3}{4} \) is the Hamiltonian of the Heisenberg exchange interaction between spins \( i \) and \( j \) with the constant added for convenience.

Since the determinant of a product of operators is equal to the product of the determinants of those operators, the requirement that the condition (2.32) hold for the sequence (2.33) implies that

$$\frac{\det U_n|_{d=0} \det U_n|_{d=2}}{\det U_n|_{d=1}} \neq 1, \tag{2.34}$$

for at least one of the \( U_n \) operations. Given that \( \det U_n = \det e^{-it_n \mathcal{H}_n} = e^{-it_n \text{Tr} \mathcal{H}_n} \), this condition can be translated into a condition on the trace of the Hamiltonian of a single pulse. If we denote the trace of \( \mathcal{H}_n \) within a sector of total spin \( d \) as \( \text{Tr} \mathcal{H}_n|_{d} \), then (2.34) implies that at least one Hamiltonian \( \mathcal{H}_n \) pulsed in (2.33) must satisfy the condition

$$\text{Tr} \mathcal{H}_n|_{d=0} - \text{Tr} \mathcal{H}_n|_{d=1} + \text{Tr} \mathcal{H}_n|_{d=2} \neq 0. \tag{2.35}$$

However, for \( \mathcal{H}_n = \mathbf{S}_{i(n)} \cdot \mathbf{S}_{j(n)} + \frac{3}{4} \) where spins \( i(n) \) and \( j(n) \) label two of the four central spins in Fig. 2.12(c), one finds that \( \text{Tr} \mathcal{H}_n|_{d=0} = 1, \text{Tr} \mathcal{H}_n|_{d=1} = 2, \) and \( \text{Tr} \mathcal{H}_n|_{d=2} = 1. \) Thus we see that

$$\text{Tr} \mathcal{H}_n|_{d=0} - \text{Tr} \mathcal{H}_n|_{d=1} + \text{Tr} \mathcal{H}_n|_{d=2} = 1 - 2 + 1 = 0. \tag{2.36}$$

It immediately follows that any pulse sequence consisting of exchange pulses between two of the four central spins in Fig. 2.12(c) cannot produce an operation of the form (2.30) and thus cannot produce a leakage-free, entangling two-qubit gate.
Lastly, we point out that if the trace condition (2.36) holds for two operators, $H_1$ and $H_2$, it trivially also holds for their sum $H_1 + H_2$. It immediately follows that our result that acting on only four spins is not sufficient to carry out an entangling two-qubit gate holds not just when the exchange interaction is pulsed in series, but also when it is pulsed in parallel (e.g. when operations of the form $e^{-it(S_1 \cdot S_2 + S_2 \cdot S_3)}$ are included). This also follows from the fact that such parallel operations can always be approximated, to any required accuracy, by sequences of operations carried out in series, as shown in Ref. [48].

### 2.4 Construction of a 25-Pulse Sequence

The pulse sequence derived in the previous section is not the most efficient sequence for carrying out an entangling two-qubit gate. As we discussed in the introduction to this chapter, Sec. 2.1, the shortest sequence for carrying out a CNOT gate up to single-qubit rotations has been found by Fong and Wandzura through a numerical search [101].

In the present section, we show that some the elements of the 39-pulse sequence of Sec. 2.3 can be extended by a new element in order to construct a new family of pulse sequences that consist of only 25 pulses [93]. As is the case for the 39-pulse sequences of the previous section and the Fong-Wandzura sequence of Ref. [101], these 25-pulse sequences act on only five of the six spins that are used to encode two qubits. In accordance with the observation described in Sec. 2.3.5, the sequences constructed below carry out entangling two-qubit gates independently of the total spin of all six spins encoding two qubits. Furthermore, the operation corresponding to these 25-pulse sequences is the same as that of the 39-pulse pulse sequences described above, i.e., it is a controlled-phase gate whose associated phase can be arbitrarily chosen.

Figure 2.13: (a) For completeness, we review the three-spin qubit encoding introduced in Sec. 2.2. Qubits are encoded into triplets of electrons with total spin $1/2$. (b) Two three-spin qubits in states $a$ and $b$, shown in a basis convenient for constructing the 25-pulse sequence in the current section. Note that this basis is slightly different from that used in Sec. 2.3 as shown in Fig. 2.2.
Figure 2.13(a) shows the three-spin qubit encoding of Ref. [46] which we use throughout this chapter. We introduce a minor change in notation compared to Sec. 2.3, which can be seen in the figure for the case of the noncomputational state $|nc\rangle$. Note that if the total spin of three spin-1/2 particles is equal to $3/2$, then the two different bases in which we first couple the leftmost or rightmost two spins are equivalent, as shown in the following equality,

$$\begin{align*}
((\bullet\bullet)a)_{3/2} &= (\bullet(\bullet)a)_{3/2} \equiv (\bullet\bullet\bullet)_{3/2}.
\end{align*}$$

(2.37)

Because of this, we simplify our notation in the following, by suppressing ovals (or parentheses) whenever possible, as for the noncomputational state shown in Fig. 2.13(a).

The basic elements used in new two-qubit gate construction shown in the current section are the same as those in the previous section, that is, they are the operations $U_3$ and $U_4$ that were introduced in Secs. 2.3.2 and 2.3.3. A key difference to the construction in Sec. 2.3, however, is the basis that use to describe the two-qubit states. For the construction below we use the basis shown in Fig. 2.13(b), which differs from the basis shown in Fig. 2.2(b) only in the particular basis choice for the qubit with state label $b$ on the right-hand side in each of these figures. This new basis in Fig. 2.2(b) will enable us to easily determine a new building block for our two-qubit gate construction.

This section is organized as follows. First, in Secs. 2.4.1, 2.4.2 and 2.4.3 we review, respectively, an exchange pulse acting on two spin-1/2 particles, the $U_3$ operation which was introduced in Sec. 2.3.2 and the $U_4$ operation that was introduced in Sec. 2.3.3. In Sec. 2.4.4, we then determine the matrix representations of these operations when acting on the Hilbert space of five spins in the basis shown in Fig. 2.13(b). In doing so, we find that a total of three different operations are useful to construct a two-qubit pulse sequence, whereas in Sec. 2.3 we only used two different operations. Finally, in Sec. 2.4.5 we then construct a 25-pulse sequence and explicitly provide its single-pulse representation.

### 2.4.1 Two-Spin Exchange Pulse

We describe the action of a Heisenberg exchange pulse of dimensionless duration $t$, as it has been defined in Sec. 2.3.1, acting on two spin-1/2 particles $S_1$ and $S_2$ with total spin $a = 0$ or 1, $(\bullet\bullet)_a$, by the time-evolution operator $\exp(-it(\mathbf{S}_1 \cdot \mathbf{S}_2 + \frac{3}{4}))$ (setting $\hbar = 1$). When evaluating this
unitary operator in the total-spin basis \( a = \{0, 1\} \) where \( a = 0 \) corresponds to the spin singlet state and \( a = 1 \) to the triplet state,\(^5\) we find

\[
U_2(t) = \begin{pmatrix}
1 & e^{-it} \\
0 & e^{it/2} \sigma_z/2
\end{pmatrix} = e^{-it/2} e^{it/2} \sigma_z/2.
\]

(2.38)

Upon defining a pseudospin with \( \uparrow = (\bullet)_0 \) and \( \downarrow = (\bullet)_1 \), this operation \( U_2 \) can be interpreted as a \( z \)-axis rotation in pseudospin space through angle \( t \) (times an overall phase factor of \( e^{-it/2} \)).

### 2.4.2 Review of Three-Spin Operation

To construct a new 25-pulse sequence we begin by reviewing two kind of pulse sequences that were introduced in Sec. 2.3 and that act on three and four spins. First, consider Fig. 2.14(a) which shows a pulse sequence acting on three spin-1/2 particles. As given in the figure, the three-dimensional Hilbert space of these spins is spanned by the states \((\bullet)_0\bullet\) with \( ac = 0, 1 \) and \( 1 \). As explained in Sec. 2.3.2, the operations corresponding to each of the three pulses of durations \( t, t, t \) in this sequence can be understood as pseudospin rotations acting on a pseudospin whose up and down states are \( \uparrow = ((\bullet)_0\bullet)_{1/2} \) and \( \downarrow = ((\bullet)_1\bullet)_{1/2} \). We used a geometric interpretation of these rotations, shown in Fig. 2.6, to explain why these pulses carry out a pseudospin rotation about the \( z \) axis, so that when evaluating the operation carried out by this sequence in the basis \( ac = \{0, 1, 1\} \), we obtain the matrix representation shown in Fig. 2.14(a). Two equations that

\(^5\)as emphasized in Sec. 2.2, since the isotropic exchange Hamiltonian is rotationally invariant we consider, for example, this three-fold degenerate \( a = 1 \) state as a single state in the two-spin Hilbert space
describe the relationship between $t$, $\bar{t}$ and $\phi$ are given in the same figure, and these equations must be solved in order to find the values for $t$ and $\bar{t}$ for a desired value of $\phi$. As opposed to the matrix representation of the operation carried out by this sequence as given in Fig. 2.5, here in the equation shown in Fig. 2.14(b) we schematically separate sectors in the Hilbert space with different values of $a = 0$ and $1$. Since this matrix is block-diagonal in $a$ and for $a = 0$ acts proportional to the identity, when using this $U_3$ operation in the following we are free to focus on the action of $U_3$ for the case of $a = 1$ while keeping track of the phase factor $e^{-it}$ that multiplies the $a = 0$ state.

We noted in Sec. 2.3.2 that for a given value of $\phi$ there are two solutions for $t$ and $\bar{t}$, one with $0 \leq t \leq \bar{t} < 2\pi$ and another with $0 \leq \bar{t} \leq t < 2\pi$. Sequences of the first kind are called short sequences, because their total duration, $2t + \bar{t}$, is shorter than that of the sequences of the second kind, called long sequences. In the following, we assume for simplicity that we always solve the equations in Fig. 2.14(a) for $t$ and $\bar{t}$ corresponding to the short sequence, and for the inverse operation we will always the long sequence with pulse durations $s$, $\bar{s}$, $s$, for which $s = 2\pi - t$ and $\bar{s} = 2\pi - \bar{t}$.

### 2.4.3 Review of Four-Spin Operation

Second, consider the pulse sequence shown in Fig. 2.14(b) whose operation we denote as $U_4$. The action of this operation, which acts on four spins $((\bullet\bullet)_a(\bullet\bullet)_b)_d$, has been discussed in detail in Sec. 2.3.3. In the pulse sequence construction of Sec. 2.3, this $U_4$ operation was always applied to the two spin pairs $(\bullet\bullet)_a$ and $(\bullet\bullet)_b$ which are also highlighted in Fig. 2.2 under the label “Four Spins,” and which are used to define the basis states of the two encoded three-spin qubits that the final two-qubit gate pulse sequence acts on. Even though in this construction, for the basis choice of Fig. 2.13(b) the same two pairs are not located directly next to each other, below in Sec. 2.4.5 we will apply the $U_4$ operation to the same spin pairs $(\bullet\bullet)_a$ and $(\bullet\bullet)_b$ which define the basis states of the qubits.

The total Hilbert space of these four particles $((\bullet\bullet)_a(\bullet\bullet)_b)_d$ which the $U_4$ operation acts on has a dimension of six, and these dimensions are distributed to the subspaces with total-spin $d = 0$ (two dimensional), $d = 1$ (three-dimensional) and $d = 2$ (one-dimensional). The sequence shown in the figure consists of three $U_3$ operations, each of which is acted on the topmost three spins and therefore necessarily conserve the quantum number $a$. As we just pointed out in the previous paragraph, this quantum number $a$ belongs to the spin pair that is used to define the basis states.
of the left qubit in Fig. 2.13(b). In fact, in the following this spin pair $(\bullet\bullet)_a$ will only be acted on by $U_3$ operations. Note that the $U_3$ operations act on the $a = 0$ subspace as a phase factor times the identity operation, as shown in Fig. 2.14(a). We will keep track of this phase and neutralize it by enacting a single-qubit on the qubit in state $a$.

From now on we can focus on the nontrivial case of $a = 1$, which we do by replacing the topmost two spins by the symbol ▲ which represents a spin-1 particle. The states in the $a = 1$ Hilbert space are given by $(▲(\bullet\bullet)_b)_d$, and in this case the two spaces for $d = 0$ and $d = 2$ are one-dimensional ($b = 1$ in each case), while the space for $d = 1$ is two-dimensional (here $b = 0$ or 1).

In Sec. 2.3.3 we identified the operations $U_3$ and $U_2$, the latter corresponding the exchange pulse that is acted on the lowermost two spins shown in Fig. 2.14(b), as pseudospin rotations the $d = 1$ Hilbert space spanned by the up and down states of the pseudospin $\uparrow = (▲(\bullet\bullet)_0)_1$ and $\downarrow = (▲(\bullet\bullet)_1)_1$. Using a geometric interpretation of the corresponding pseudospin rotations of this pulse sequence, as shown in Fig. 2.8, we were able to determine the action of this pulse sequence which is, in essence, to diagonalize the matrix representation of the central $U_3(\phi)$ operation by mapping its rotation axis in pseudospin space to the $z$ axis. The corresponding matrix representation of this sequence in the basis $bd = \{10|01|11, 12\}$ is then that shown in Fig. 2.14(b). In this matrix we schematically separate out the one-dimensional $b = 0$ sector where $U_4$ acts as the identity. Because $U_4$ acts trivially on the $b = 0$ state, in what follows we will be allowed to separate the discussion of $b = 0$ and the non-trivial case of $b = 1$.

As we have seen in Sec. 2.3.4, the operations $U_3$ and $U_4$ as given here can be acted on five of the six spins encoding two qubits to form a pulse sequence of 39 pulses that carries out a controlled-phase gate. In the following, we will basically repeat this exercise but making use of three different unitary operations, rather than only two operations as it was the case in Sec. 2.3.4.

### 2.4.4 New Operations Acting on Five Spins

We now construct a new two-qubit gate pulse sequence that carries out a controlled-phase gate by acting on five of the six spins that encode two three-spin qubits, $((\bullet\bullet)_a(\bullet\bullet)_b)_f$, whose state is also shown in Fig. 2.13(b). Since the total spin of both qubits can only be either 0 or 1, the total spin of these five particles can only be either $f = 1/2$ or $3/2$. The relevant Hilbert space of these particles is five-dimensional for total spin $f = 1/2$ and four-dimensional for $f = 3/2$. 

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Figure 2.15: One $U_4$ operations and two $U_3$ operations, one of which we denote as $\tilde{U}_3$ to be able distinguish them, which are acted on five spin-1/2 particles.

Figure 2.15 shows three different operations, one of which is a $U_4$ operation and the other two are $U_3$ operations, acting on the five spins highlighted in Fig. 2.13(b). We denote the lowermost $U_3$ operation, which acts on the topmost $\triangle$ and central $\bullet$, as $\tilde{U}_3$ for the sole purpose to distinguish it from the topmost $U_3$ operation, which acts on the lowermost $\triangle$ and $\bullet$. Crossing particle-lines imply that the spin-1/2 particle, $\bullet$, and the lower effective spin-1 particle, $\triangle$, exchange positions. This operation that may be carried out by two SWAP pulses$^6$ as shown in Fig. 2.16. Each of these pulse sequences is applied in such a way that the quantum numbers $a$ and $b$ are conserved. As shown in Fig. 2.15, we are therefore able to simplify the Hilbert space of these five spins by first focusing on the case of $a = b = 1$ by replacing each spin pair with total spin $a$ and $b$ by an effective spin-1 particle denoted as $\triangle$,

$$\left((\bullet\bullet)_a(\bullet\bullet)_b\right)_c \rightarrow (\triangle\triangle)_c. \tag{2.39}$$

The effective four-dimensional Hilbert space of these particles is then spanned by the states with $cf = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}$ and $\frac{3}{2}, \frac{5}{2}, \frac{7}{2}$. To properly describe the action of each of the operations of Fig. 2.15

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$^6$For the convention of the dimensionless measure of duration, $t$, according to Eq. (2.38) a SWAP pulse has duration $t = \pi$. 

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we define a pseudospin whose up and down states, respectively, are given by $|f\rangle = (\uparrow\uparrow)_{1/2}f$ and $|\downarrow f\rangle = (\uparrow\downarrow)_{3/2}f$ for each total-spin sector with either $f = 1/2$ or $3/2$.

To understand the effect of interchanging a spin-1/2, $\bullet$, and an effective spin-1, $\uparrow$, consider these two particles in the state $(\bullet\uparrow)_{e}$ with total spin $e = 1/2$ or $3/2$. A trivial observation is that exchanging these two particles results in an “active” change of basis from $(\bullet\uparrow)_{e}$ to a new basis, $(\uparrow\bullet)_{e}$. At the same time, however, the different states with $e = 1/2$ and $3/2$ get multiplied by a different sign. To see this, in Fig. 2.16 we temporarily replace the effective spin-1 particle, $\uparrow$, by two spin-1/2 particles with total spin 1, $(\bullet\bullet)_{1}$. In the figure we then give the single-pulse representation that carries out the exchange of $\bullet$ and $\uparrow$, which consists of two swap pulses. This sequence can be easily evaluated if the total spin is equal to $e = 3/2$, because in this case the three spins are in the state $(\bullet\bullet\bullet)_{3/2}$. Since in this case, as shown in Eq. (2.37), either spin pair has total spin 1, either swap pulse, according to Eq. (2.38), applies a factor of $e^{i\pi} = -1$ to the state. The result of applying two of these pulses is therefore to multiply the state $(\bullet\bullet\bullet)_{3/2}$ by +1, as shown in the figure. Conversely, if $e = 1/2$, we may consider the two-dimensional Hilbert space of three spins, $(\bullet\bullet\bullet)_{1/2}$, and enact the two swap pulses on the $a = 1$ state. The matrix representation of this operation can be obtained by direct calculation. The matrix for the basis change

$$((\bullet\bullet\bullet)_{1/2} \xrightarrow{F_{1}} (\bullet\bullet\bullet)_{1/2})$$

is given by

$$F_{1} = \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & 1/2 \end{pmatrix}$$

which has also been introduced in Sec. 2.3.2. Comparing the matrix due to the exchange pulses with $F$, one will find indeed that the effect that the exchange pulses have on the three-spin state $((\bullet\bullet\bullet)_{a=1/2})$ is equal to the effect of $F$ up to a minus sign, as shown in Fig. 2.16.

We can now determine the action due to the exchange of the central spin-1/2 particle, $\bullet$, and the lowermost spin-1 particle, $\uparrow$, shown as crossing particle lines in Fig. 2.15, on the pseudospin $|f\rangle$ defined above. First, note that by this exchange the basis $(\uparrow\uparrow\bullet)_{e}f$ get transformed to the basis $(\uparrow\downarrow\bullet)_{e}f$. Second, we need to take into account that states with different values of $e$ get multiplied by different factors of +1 or −1, see Fig. 2.16. The corresponding matrix in the $e = \{1/2, 3/2\}$ basis can be rewritten as $\begin{pmatrix} -1 & 1 \end{pmatrix} = e^{-i\pi/2}e^{-i\pi/2}\sigma/2$. We can thus describe the action of this exchange as a change from the pseudospin $|f\rangle$ to another pseudospin defined as $\uparrow f = (\uparrow\uparrow\bullet)_{e=1/2}f$ and
Figure 2.16: Explicit pulse-sequence consisting of two swap pulses that can be used to exchange a spin-1, ▲, and a spin-1/2, •, which are initially in the state ((●●)₁)ᵣ → (▲●)ᵣ. As explained in the main text, the process of exchanging these two particles is associated with a change of basis and a z-axis rotation through angle π.

\[ \downarrow f = (▲(●●)ᵣ=3/2) f \] (the same pseudospin has been used in Sec. 2.3.4), followed by a rotation about the (negative) z axis within this pseudospin space through an angle π. Equivalently, this action can be represented by the following set of equations,

\[
\begin{align*}
(▲(●●)ᵣ) f & \rightarrow e^{-i\pi/2} e^{-i\pi \sigma_z/2} (▲(●●)ᵣ) f \\
\Leftrightarrow (|f, 1\rangle) & \rightarrow e^{-i\pi/2} e^{-i\pi \sigma_z/2} (|f, 1\rangle).
\end{align*}
\]  

Note that in Fig. 2.15 these exchange operations appear on both sides of the operations \( U₃ \) and \( U₄ \), and ensure that each of these operations conserves the quantum numbers \( a \) and \( b \) by carrying out the change of basis (2.42). We will find that the z-axis rotation through angle π, which is associated with this basis change, will only have a nontrivial effect on the operation \( U₄ \).

We now turn to evaluating the operations shown in Fig. 2.15. Beginning with the topmost \( U₃ \) operation which acts on the central spin-1/2 particle • and the lowermost spin-1 particle ▲, first note that we can read the matrix representation in the basis \((▲(●●)ᵣ) f\) directly from Fig. 2.14(a) for the case of \( a = 1 \). We find that in the pseudospin space \( ↑ f \) this operation \( U₃ \) carries out a z-axis rotation through angle \( t \). The effect of the exchanges of the particles • and the lowermost ▲ located to the left and the right of \( U₃ \) is then to actively carry out a basis change that maps the pseudospin \( ↑ f \) to the pseudospin \( |f, 1\rangle \), as shown in Eq. (2.42). Since the \( U₃ \) operation itself carries out a z-axis rotation in pseudospin space, the z-axis rotations through angle π associated with the basis change commute with \( U₃ \) and cancel one another. The action of the \( U₃ \) operation flanked by the exchanges of • and ▲ is therefore to carry out a z-axis rotation through angle \( t \) in pseudospin space \( |f, 1\rangle \) for \( f = 1/2 \) and 3/2, as shown in Fig. 2.15.

We can read the action of the operation \( U₄ \) in the basis \((▲(●●)ᵣ) f\) from Fig. 2.14(b) for the case of \( b = 1 \) to find that, in the total spin \( f = 1/2 \) sector, then \( U₄(t) \) carries out a z-axis rotation.
through angle $t$ in the basis with $d = \{0, 1\}$,

$$U_{4,d}^{f=1/2}(t) = \begin{pmatrix} 1 & e^{-it} \\ e^{-it}& 1 \end{pmatrix} = e^{-it/2}e^{it\hat{z}\cdot\sigma/2}$$

(2.43)

while in the $f = 3/2$ sector it acts as the identity times a factor of $e^{it}$,

$$U_{4,d}^{f=3/2}(t) = \begin{pmatrix} e^{-it} & 0 \\ 0 & e^{-it} \end{pmatrix} = e^{-it}1.$$  

(2.44)

Here, as in Sec. 2.3, the notation $U_{4,d}^{f=1/2}$ refers to the $U_{4,d}$ operation whose matrix representation is given in the $d$-basis and restricted to the sector of total spin $f = 1/2$. In Sec. 2.3.4, when transforming to the basis $(\uparrow(\uparrow\bullet)e)_f$ we found that the action of $U_{4,d}$ in the case of $f = 1/2$ on the pseudospin $\uparrow_f$ is given by $e^{-it/2}e^{it\hat{n}_2\cdot\sigma/2}$ [see Eq. (2.21)] which performs a rotation about the vector $\hat{n}_2$, which makes an angle of $\cos^{-1}(-1/3)$ with the $z$ axis. Similar to the operation $U_3$ discussed above, the exchanges of $\bullet$ and the lowermost $\uparrow$ on both sides of $U_{4,d}$ in Fig. 2.15 then carry out an active basis change to the pseudospin $\uparrow_f$. While the action of $U_3$ in pseudospin space was to perform a $z$-axis rotation, however, the rotation of $U_{4,d}$ in the pseudospin space is about an axis that is not parallel to the $z$ axis, because of which the $z$-axis rotations through angle $\pi$ associated with the exchanges on either side of $U_{4,d}$ [see Eq. (2.42)] alter the rotation axis,

$$U_{4,d}^{f=3/2}(t) = (e^{-i\pi/2}e^{-i\pi\hat{n}_2\cdot\sigma/2})(e^{-it/2}e^{it\hat{n}_2\cdot\sigma/2})(e^{-i\pi/2}e^{-i\pi\hat{n}_2\cdot\sigma/2}) = e^{-it/2}e^{it\hat{n}_3\cdot\sigma/2}.$$  

(2.45)

The result of the two $z$-axis rotations through angle $\pi$ is to reflect the vector $\hat{n}_2 = (-2\sqrt{2}/3, 0, -1/3)$ about the $z$ axis to the vector $\hat{n}_3 = (2\sqrt{2}/3, 0, -1/3)$ which, of course, as shown in Fig. 2.15, also makes an angle of $\cos^{-1}(-1/3)$ with the $z$ axis. In the $f = 3/2$ sector, the basis changes have no effect on the matrix representation of $U_{4,d}$ as given in Eq. (2.44) since this matrix it is proportional to the identity. The matrix representation of $U_{4,d}$ on the pseudospin $\uparrow_f$ in both $f = 1/2$ and 3/2 sectors is shown in Fig. 2.15.

The lowermost operation shown in Fig. 2.15, $\tilde{U}_3$, is a $U_3$ operation that acts on the topmost $\uparrow$ and the central $\bullet$. The matrix representation of this operation can be found most easily in the basis $((\uparrow\bullet)e',\uparrow)_{1/2}$. From Fig. 2.14(a) for the case of $a = 1$ we find that its action, independent of $f$, is that of a $z$-axis rotation through angle $t$ for the state ordering $e' = \{1/2, 3/2\}$,

$$\tilde{U}_{3,e'}^{f=1/2}(t) = \begin{pmatrix} 1 & e^{-it} \\ e^{-it} & 1 \end{pmatrix} = e^{-it/2}e^{it\hat{z}\cdot\sigma/2}.$$  

(2.46)
We calculate its action onto the pseudospin space \( f = \frac{1}{2} \) by performing the basis change

\[
((\blacklozenge \bullet) e')_{1/2} \rightarrow (\blacklozenge (\bullet \blacklozenge) e)_{1/2}
\]

(2.47)

with the matrix

\[
F = \begin{pmatrix}
-1/3 & 2\sqrt{2}/3 \\
2\sqrt{2}/3 & 1/3
\end{pmatrix}
\]

(2.48)

where \( \hat{f} = 2\sqrt{2}/3, 0, -1/2 \). The matrix elements of \( F \) are the recoupling coefficients

\[
F = \langle ((\blacklozenge \bullet) e')_{1/2}|(\blacklozenge (\bullet \blacklozenge) e)_{1/2}\rangle.
\]

This matrix \( F \) performs the map (2.47) from \( e' = \{ \frac{1}{2}, \frac{3}{2} \} \) to \( e = \{ \frac{1}{2}, \frac{3}{2} \} \), and since \( F^{-1} = F \) we can then write

\[
\tilde{U}_{3,e}(t) = F \tilde{U}_{3,e'}^{f=1/2}(t) F = e^{-it/2} e^it\hat{n}_4 \cdot \sigma/2
\]

(2.49)

to find that in the action of \( \tilde{U}_3 \) on the pseudospin \( f = 1/2 \) is given by a rotation about an axis

\[
\hat{n}_4 = 2\hat{f}(\hat{f} \cdot \hat{z}) - \hat{z} = (\frac{4\sqrt{2}}{9}, 0, -\frac{7}{9})
\]

which makes an angle of \( \cos^{-1}(-7/9) \) with the z axis, as shown in Fig. 2.15. A similar analysis can be performed to determine the rotation axis of this \( U_3 \) operation in the \( f = 3/2 \) sector. However, we will find that the exact matrix representation for \( f = 3/2 \) is irrelevant for what follows and we therefore describe the matrix representation in Fig. 2.15 formally by a pseudospin rotation through angle \( t \) about an axis denoted \( \hat{n}_5 \) which requires no further specification. Figure 2.15 shows the corresponding matrix representation of the operation \( \tilde{U}_3 \).

**2.4.5 Family of 25-Pulse Sequence**

Similar to Sec. 2.3.4, we now construct a new two-qubit gate pulse sequence using the operations shown in Fig. 2.15. Figure 2.17(a) summarizes the construction of this sequence whose operation on the Hilbert space spanned by the states \((\blacklozenge (\bullet \blacklozenge) e)_{f}\), as also shown in Eq. (2.39), we denote \( U_5 \). The sequence shown in the figure is built of a pair of \( \tilde{U}_3 \) operations, a pair of \( U_3 \) operations and a single \( U_4 \) operation, in the latter two cases including the exchanges of the particles \( \bullet \) and \( \blacklozenge \) as given in Fig. 2.15. Each of these exchange operations on either side of \( U_4 \) cancels with one of the (opposite) exchange operations located next to the neighboring \( U_3 \) operations, and only the remaining exchange operations are shown in Fig. 2.17(a). The operations due to all of these operations on the Hilbert space (2.39) are then those shown in Fig. 2.15. The unitary operation of
this sequence can therefore be written as

\[ U_5(\phi) = \bar{U}_3(s_7)U_3(s_6)U_4(\phi)U_3(t_6)\bar{U}_3(t_7) \]

\[ = S^{-1}U_4(\phi)S \]  \hspace{1cm} (2.50)

with \( s_6 = 2\pi - t_6 \) and \( s_7 = 2\pi - t_7 \). From Eq. (2.50) it is evident that the \( U_5 \) sequence is the result of a similarity transformation carried out by the operation \( S = U_3(t_6)\bar{U}_3(t_7) \).

The operation \( U_5(\phi) \) of Fig. 2.17(a) is designed to apply a phase factor \( e^{i\phi} \) to the states \( (\blacktrianglebullet\blacktriangle)_{ef} \) with \( ef = \{1/2, 3/2\} \) and \( \{3/2, 3/2\} \). In the \( f = 3/2 \) sector, the operation \( U_4(\phi) \), as shown in Fig. 2.15, acts as the identity times \( e^{i\phi} \). Since here, accordingly, the similarity transformation in Eq. (2.50) has no effect it follows that \( U_5(\phi) \) multiplies every state in the \( f = 3/2 \) sector by a phase factor and thus also, in particular, the state \( (\blacktrianglebullet\blacktriangle)_{e=1/2}^{f=3/2} \).

We now focus on the nontrivial case of \( f = 1/2 \). Interpreting the action of the three different operations used in this sequence as rotations on the pseudospin \( |1/2\rangle \), we aim to rotate the rotation vector of \( U_4(\phi) \), \( \hat{n}_3 \), via the similarity transformation to the \(-z\) axis. This is because after carrying out such a transformation the matrix representation of \( U_5 \) in this sector in the basis \( e = \{1/2, 3/2\} \) will be given by

\[ U_{5,e=1/2}^{f=1/2}(\phi) = e^{-i\phi/2}e^{i\phi/2}(-\hat{z})/\sigma_{f=1/2} = \begin{pmatrix} e^{-i\phi} & 0 \\ 0 & 1 \end{pmatrix}, \]  \hspace{1cm} (2.51)
which indeed multiplies the state $\left(\Delta (\bullet \Delta)_{\ell}\right)_{f}$ by a phase factor of $e^{-i\phi}$.

To understand how the similarity transformation carried out by $S = U_{3}(t_{6})\tilde{U}_{3}(t_{7})$, as defined in Eq. (2.50), accomplishes the map of $\hat{n}_{3}$ to $-\hat{z}$, consider the two intersecting cones in Fig. 2.17(a). The darker cone in the figure describes all possible outcomes when rotating the vector $\hat{n}_{3}$ about the $z$ axis. Similarly, the lighter cone describes the possible outcomes when rotating the vector $-\hat{z}$ about the $n_{4}$ axis. As shown, the similarity transformation is carried out in the following two steps. First, an application of $U_{3}(t_{6})$ rotate $\hat{n}_{3}$ about the $z$ axis through an angle $t_{6}$ to the intersection of the two cones. In the second step, an application of $\tilde{U}_{3}(t_{7})$ rotates the resulting vector about the $n_{3}$ axis through angle $t_{7}$ to $-\hat{z}$. A simple calculation yields these values of these two rotations angles to be

$$t_{6} = \cos^{-1}\left(-\frac{n_{4,z}(1 + n_{3,z})}{n_{4,n_{3},x}}\right) = \cos^{-1}(-7/8)$$

and

$$t_{7} = \cos^{-1}\left(-\frac{n_{3,z} + n_{4,z}^{2}}{n_{4,x}^{2}}\right) = \cos^{-1}(-11/16),$$

where $n_{i,x}$ and $n_{i,z}$ are the $x$ and $z$ components, respectively, of unit vector $\hat{n}_{i}$ for $i = 3, 4$.

The matrix representation of $U_{5}$ is therefore given by that of Eq. (2.51) for $f = 1/2$ and, as discussed above, equal to $e^{i\phi}$ times the identity operation for $f = 3/2$. The combined matrix representation of this operation $U_{5}$ is given in Fig. 2.17(a). Figure 2.17(b) shows that this operation, when acted on five of the six spins that encode two qubits [see also Fig. 2.13(b)] carries out a controlled-phase gate. To prove this, it is sufficient to determine the action of $U_{5}$ on the four encoded qubit states that define the standard basis, that is, the two-qubit states with $ab = 00, 01, 10$ and 11.

Above we have already established that if $a = 1$ and $b = 1$, the five-spin states (2.39) are multiplied by a phase factor of $e^{-i\phi}$. For the last case of $ab = 11$, in Sec. 2.3.4 we have expanded the two-qubit states shown on the left-hand side of Fig. 2.13(b) into the basis shown on the right-hand side of the same figure. From this expansion in Eqs. (2.23) and (2.24) it is clear that since $U_{5}(\phi)$ multiplies both $f = 1/2$ and $3/2$ states with $e = 1/2$ by the phase factor $e^{-i\phi}$, it also multiplies the two-qubit states with $ab = 11$ by the same factor.

We discussed in Sec. 2.4.3 that the two spins $(\bullet)$, which define the basis states of the left qubit shown in Fig. 2.13(b), only get acted on by $U_{3}$ operations, and since such $U_{3}$ acts as the identity times a phase factor on all $a = 0$ states [see its matrix presentation given in Fig. 2.14(a)],
Figure 2.18: Single-pulse representation of the sequence $U_5$ acting on two encoded three-spin qubits. Red pulses depend on the phase $\phi$ which determines the controlled-phase gate, and black pulses are independent of $\phi$. The pulse durations which do not depend on $\phi$ (some of which were also given in Sec. 2.3.4) are $t_4 = 2\pi/3$, $s_4 = 4\pi/3$, as well as $t_1 = 1.34004$, $t_8 = 1.47560$ and $t_9 = 1.6467482652$ (obtained by solving for the short sequences for $U_3(t_4)$, $U_3(t_6)$ and $U_3(t_7)$ see Sec. 2.3.2), together with those obtained from the relations $\tan(t_i/2)\tan(\bar{t}_i/2) = -2$ and $\bar{t}_i + \bar{s}_i = t_i + s_i = 2\pi$ for $i = 1, 8, 9$. The times $t$ and $\bar{t}$ depend on $\phi$ and are found by solving for the short or long sequence for $U_3(\phi)$.

The $a = 0$ two-qubit subsector simply gets acted on by an operation that is proportional to the identity operation. In the case of the sequence for $U_5$ shown in Fig. 2.17(a), for $a = 0$ the similarity transformation therefore has no effect on the operation $U_4$. Not only is the similarity transformation of the identity without obvious effect, but it is further ensured that this similarity transformation does not multiply the $a = 0$ (or $b = 0$) states by an overall phase factor. This is because in Sec. 2.4.2 we made the choice to always solve for short operations $U_3(t)$ and use the long operations for their inverses $U_3(s)$ where $s = 2\pi - t$, in which case the phase factors of $U_3$ and its inverse on the $a = 0$ states, as given in Fig. 2.14(a), are equal and of opposite sign.

Figure 2.17(b) shows, as we just worked out, that the operation $U_5$ applied to two encoded three-spin qubits enacts an entangling two-qubit gate. Upon including the single-qubit rotation of appropriate duration $t_a$ on the qubit with state label $a$, this gate acts the identity operation on the two-qubit states with $ab = 00$, 01 and 10, while it multiplies the state with $ab = 11$ by the phase factor $e^{-i\phi}$. As given in Fig. 2.17(b), the according two-qubit gate is thus a controlled-phase gate.

The explicit single-pulse sequence corresponding to the operation of Fig. 2.17 is shown in Fig. 2.18. This sequence is obtained by first replacing the operation $U_4$ in Fig. 2.17(a) by its sequence given in Fig. 2.14(b), which consists of single pulses and $U_3$ operations, and then replacing all $U_3$ sequences by their single-pulse representations as given in Fig. 2.14(a). Furthermore,
the line crossings shown in Fig. 2.17(a) that indicate the exchange of spins are replaced by their single-pulse representation given in Fig. 2.16.

Finally, we need to determine the pulse duration \( t_a \) of the single-qubit operation as shown in Fig. 2.17(b). Given that the central three pulses, shown in red in Fig. 2.18, corresponding to the central \( U_3(\phi) \) operation, which itself is in the center of the \( U_4(\phi) \) operation of Fig. 2.17(a), is carried out by the three pulses \( t, \bar{t}, t \), this central \( U_3 \) operation multiplies the \( a = 0 \) two-qubit sector by a factor of \( e^{-i\bar{t}} \) [see the matrix representation of \( U_3 \) given in Fig. 2.14(a)]. Since, as discussed above, for every \( U_3 \) operation besides the one in the center there is also the corresponding inverse, there is no further resulting phase factor acting on the \( a = 0 \) sector. In order to undo the phase factor of \( e^{-i\bar{t}} \) that results from the central \( U_3 \) operation, we enact a single-qubit rotation at the end of the two-qubit gate sequence in form of an exchange pulse of duration \( t_a = \bar{t} \) on the two spins \((\bullet\bullet)_a\) of the upper qubit.

When counting the total number of pulses shown in Fig. 2.18 one will find that there are 27 pulses, not taking the single-qubit rotation pulse into account. This number reduces to 25 because the two swap-pulses acting on the lowermost two spins can be combined with their respective neighboring pulses of durations \( t_9 \) and \( s_9 \).

This 25-pulse sequence as well as the 39-pulse sequence constructed in Sec. 2.3 are significantly longer than both the 19-pulse DiVincenzo et al. [46] sequence (which only carries out a gate locally equivalent to \textsc{cnot} in the total spin \( g = 1 \) sector) and the 18-pulse Fong and Wandzura[101] sequence (which, like our sequence, carries out a gate locally equivalent to \textsc{cnot} in both the total \( g = 0 \) and \( g = 1 \) sectors) as well as the related 16- and 14-pulse sequences for geometries other than linear arrays [114]. Nevertheless, we believe our two-qubit gate construction is of interest, because it introduces new methods for finding pulse sequences acting on large Hilbert spaces by effectively reducing the size of this Hilbert space at each stage of the construction.

### 2.5 Derivation of the Fong-Wandzura Sequence

To assess any quantum computation scheme one ultimately needs to know the minimal cost of carrying out quantum gates. For exchange-only quantum computation with pulse sequences, single-qubit gate sequences are theoretically understood but there is little true understanding regarding optimization of two-qubit gate sequences. The main difficulty is the constraint of no leakage
Figure 2.19: (a) Once again, we review the three-spin encoding first shown in Sec. 2.2, for logical qubit states with total spin 1/2, $|a\rangle$ with $a = 0, 1$, and noncomputational state with total spin 3/2, $|nc\rangle$. (b) Two qubits in states $a$ and $b$ and a diagram highlighting the five rightmost spins with total spin $f = 1/2$ or 3/2. Note that the basis of these spins is slightly different from that shown in Fig. 2.2 but the same as the one shown in Fig. 2.13.

In this section we present an analytic construction of a class of pulse sequences that carry out two-qubit gates for exchange-only quantum computation [92]. These sequences are built out of smaller sequences that act on only four spins and satisfy a certain constraint. We then show that when the most efficient of these smaller sequences is used the result is equivalent to the Fong-Wandzura sequence. Our guiding principle throughout is to avoid as much as possible complicated calculations and use only the most basic facts about quantum spin. Actually, the only essential ingredients in our construction are the familiar triangle rule for adding total spin quantum numbers,

$$s_1 \otimes s_2 = |s_1 - s_2|, |s_1 - s_2| + 1 \cdots, s_1 + s_2,$$

and the fact that interchanging two spin-$s$ particles with total spin $S_{tot}$ results in a phase factor of $(-1)^{2s-S_{tot}}$.

Figure 2.19(a) shows the three-spin qubit encoding used above, and in Fig. 2.19(b) we highlight the five spin-1/2 particles that we choose to be the spins that the Fong-Wandzura sequence acts on. This basis choice for the two-qubit system is the same as that of Sec. 2.4 but differs slightly from that of Sec. 2.3.
2.5.1 Elevation of a Pulse Sequence

Consider the exchange Hamiltonian $\mathcal{H} = J \mathbf{S}_i \cdot \mathbf{S}_j$ acting on two spin-1/2 particles (●●)$_a$ whose Hilbert space is spanned by the two states with total spin $a = 0$ and 1. (Because only total spin quantum numbers are relevant in our analysis, we treat, for example, the three-fold degenerate $a = 1$ state as a single state.) Pulsing this Hamiltonian for a duration measured in units of $1/(\pi J)$, so that the product of the time and the exchange coupling is given by a dimensionless variable that we denote as $t$ ($\hbar = 1$) up to a factor of $\pi$, results in the time evolution operator (up to an irrelevant overall phase factor),

$$U_{ij}(t) = \text{diag}(1, e^{-i\pi t}),$$

where the matrix representation is given in the $a = \{0, 1\}$ basis. We take $t \in [0, 2)$ for which the inverse pulse has duration $2 - t$. Note that the choice for the dimensionless measure of pulse duration in this section is different from how it was used in Secs. 2.3 and 2.4 as defined in Sec. 2.3.1.
Two exchange pulses square to the identity and play a fundamental role in our construction. The durations of these pulses, which we denote \( r \), can only be either 0 or 1, and we refer to them as \( r \)-pulses. For \( r = 0 \) an \( r \)-pulse is simply the identity, while for \( r = 1 \) it is a SWAP operation, which is equivalent to physically exchanging two spins. [For the phase convention of Eq. (2.55), a SWAP pulse is equivalent to carrying out a physical particle exchange and multiplying the resulting state by \(-1\).] Figure 2.20(a) shows an \( r \)-pulse acting on two spins in the state \((\bullet\bullet)_{a}\) using standard notation with exchange pulses represented by double arrows labeled by duration. The corresponding matrix representation of the resulting operation, also given in Fig. 2.20(a), shows that applying an \( r \)-pulse multiplies the \( a = 0 \) state by 1 and the \( a = 1 \) state by \( m \), where \( m = 1 \) or \( m = -1 \) for \( r = 0 \) or \( r = 1 \), respectively. In both cases \( m^2 = 1 \), reflecting the fact that the \( r \)-pulses square to the identity.

A pulse sequence that acts on three spins and consists of three \( r \)-pulses (with either \( r = 0 \) or \( 1 \) acting on the bottom two spins and two explicit SWAP pulses acting on the top two spins is shown in Fig. 2.20(b). For \( r = 0 \) the two explicit SWAP pulses square to the identity. For \( r = 1 \) the sequence consists of five SWAP pulses which, when viewed as spin permutations, are readily seen to be equivalent to a single SWAP pulse acting on the top two spins. In both cases, the effect of the sequence is to multiply the state \(((\bullet\bullet)_{a}\bullet)_{c}\) by 1 if \( a = 0 \), and \( m \) if \( a = 1 \), regardless of the value of \( c \), where, as in Fig. 2.20(a), \( m = 1 \) or \( m = -1 \) for \( r = 0 \) or \( r = 1 \), respectively. The corresponding matrix representation is also given in Fig. 2.20(b).

We seek pulse sequences which act on the five spins \(((\bullet\bullet)_{a}(\bullet(\bullet\bullet)_{b})_{1/2})_{f}\) highlighted in Fig. 2.19(b) and carry out leakage-free two-qubit gates. For reasons that will become clear we refer to the qubit with state label \( a \) as the control qubit and the qubit with state label \( b \) as the target qubit. Our construction is based on using a smaller sequence which acts on the four rightmost spins in Fig. 2.19. This smaller sequence carries out an operation we denote \( \hat{R} \) which, as seen shortly, is closely related to an \( r \)-pulse. One requirement we place on \( \hat{R} \) is that it not result in any leakage of the target qubit into its noncomputational state. We can therefore work within an effective Hilbert space in which the three spins encoding the target qubit are replaced by a single effective spin-1/2 particle,

\[
(\bullet(\bullet\bullet)_{b})_{1/2} \rightarrow \bigstar.
\]  

(2.56)

Matrix elements of operations acting on any collection of spins including \( \bigstar \) are then elevated from numbers to \( 2 \times 2 \) blocks that act on the Hilbert space of the target qubit hidden within \( \bigstar \).
We require that when \( R \) is applied to the state \((\star \star)\) it act on the target qubit with the identity \( \mathbb{1} \) if \( d = 0 \), and a matrix \( M \), with \( M^2 = \mathbb{1} \), if \( d = 1 \), as also shown in the corresponding matrix representation of \( R \) given in Fig. 2.20(c). Such \( R \) operations can be viewed as generalized \( r \)-pulses where the matrix elements 1 and \( m \), with \( m^2 = 1 \), of Fig. 2.20(a) have been elevated to the \( 2 \times 2 \) matrices \( \mathbb{1} \) and \( M \), with \( M^2 = \mathbb{1} \) in Fig. 2.20(c).

This view of \( R \) as an elevated \( r \)-pulse suggests the five-pulse sequence of Fig. 2.20(b) can also be elevated to the sequence shown in Fig. 2.20(d). This sequence acts on the effective Hilbert space spanned by the states \(( (\star \star)_{a} \star)_{f} \) with \( af = 0^1 \frac{1}{2}, 1^1 \frac{3}{2} \) and \( 1^3 \frac{3}{2} \) and consists of three \( R \) operations acting on the central spin and the effective spin \( \star \) and two \textsc{swap} pulses acting on the top two spins. The only \( 2 \times 2 \) block element in the matrix representation of \( R \) which is not proportional to the identity is \( M \). Because \( M^2 = \mathbb{1} \), when evaluating the matrix representation for the full sequence, each block matrix element must be of the form \( \alpha_0 \mathbb{1} + \alpha_1 M \). The coefficients \( \alpha_0 \) and \( \alpha_1 \) for each block element are completely determined by the two cases \( M = \pm \mathbb{1} \), which are equivalent to the cases \( m = \pm 1 \) in Fig. 2.20(b). It follows that the matrix representation of the operation carried out by this sequence in the effective \( af = \{ 0^1 \frac{1}{2}, 1^1 \frac{3}{2}, 1^3 \frac{3}{2} \} \) basis is that given in Fig. 2.20(d), i.e. an elevated version of the matrix shown in Fig. 2.20(b). To prove this result we have only used the fact that \( M^2 = \mathbb{1} \). It therefore holds not just for the straightforward cases \( M = \pm \mathbb{1} \), but also for any matrix of the form \( M = \hat{n} \cdot \sigma \) where \( \hat{n} \) is a real-valued unit vector and \( \sigma = (\sigma_x, \sigma_y, \sigma_z) \) is the Pauli vector.

The pulse sequence shown in Fig. 2.20(d) acting on the two qubits of Fig. 2.19 applies the identity \( \mathbb{1} \) to the target qubit when the state of the control qubit is \( a = 0 \), and applies the matrix \( M \) to the target qubit when the state of the control qubit is \( a = 1 \), regardless of the value of \( f \). The matrix representation of the operation carried out by this sequence can then be given in the standard two-qubit basis \( ab = \{ 00, 01, 10, 11 \} \) as

\[
U_{2\text{qubit}} = \text{diag}(\mathbb{1}, M).
\] (2.57)

For \( M = \pm \mathbb{1} \) the resulting gate is either the identity or a logical \textsc{swap} gate acting on the encoded qubits, neither of which are entangling gates. However, for \( M = \hat{n} \cdot \sigma \) the sequence enacts a leakage-free controlled-(\( \hat{n} \cdot \sigma \)) gate which is equivalent to a \textsc{cnot} gate (for which \( \hat{n} = \hat{x} \)), up to single-qubit rotations.
Figure 2.21: Constructing a pulse sequence for $R$. (a) Constraint which must be satisfied by an operation, $V$, used in the construction. (b) Sequence in which $V$, its inverse, and two SWAP pulses are used to carry out an $R$ operation. (c) Evaluation of the matrix element (2.60) for the case $t_1t_2 = 11$, as described in the text. (All quantum numbers are the same as those in (a), but are omitted for readability.) (d) One of two two-pulse solutions of (a) for $V$ which can be used to construct $R$ using (b).

2.5.2 A New Class of Two-Qubit Gate Pulse Sequences

Abandoning the notation $\star$ we now consider $R$ acting on the four-spin Hilbert space spanned by the states $(\bullet(\bullet)_{(\bullet)_{c}})_{d}$ where, since $c$ is initially $1/2$, $d$ can only be either $0$ or $1$. The requirements on $R$ needed to construct a controlled-$\hat{n}\cdot\sigma$ gate are that it must i) preserve the quantum number $c$, and ii) in the restricted Hilbert space with $c = 1/2$, have the form shown in Fig. 2.20(c) with $M = \hat{n}\cdot\sigma$.

To construct a sequence for $R$ we introduce a new operation $V$ which satisfies the constraint

$$\langle((\bullet\bullet)_{1}(\bullet\bullet)_{1})_{1}|V|((\bullet\bullet)_{3/2})_{1}\rangle = 0 \tag{2.58}$$

depicted in Fig. 2.21(a). As shown below, inserting any $V$ satisfying Eq. (2.58) into the sequence shown in Fig. 2.21(b) results in an $R$ operation with $M = \hat{n}\cdot\sigma$. Letting $U_{ij}(t)$ denote an exchange pulse of duration $t$ acting on spins $i$ and $j$, as defined in Eq. (2.55), the sequence for $R$ can be written $V^{-1}U_{12}(1)U_{34}(1)V$, using the spin labeling of Fig. 2.21(b). The matrix representation of the central two SWAP pulses $U_{12}(1)U_{34}(1)$ in the $((\bullet\bullet)_{b'}(\bullet\bullet)_{b})_{d}$ basis with state ordering $bb'd =$

82
\( \{00, 110|011, 101, 111\} \) is,

\[
U_{12}(1)U_{34}(1) = \text{diag}(1, 1| -1, -1, 1).
\] (2.59)

In the \( d = 0 \) sector \( U_{12}(1)U_{34}(1) \) acts as the identity, and thus \( R \) also acts as the identity since \( V \) and \( V^{-1} \) cancel one another. In the \( d = 1 \) sector, Eq. (2.58) implies that \( V \) maps the \( c = 3/2 \) state \( (\bullet(\bullet\bullet)_3/2)_1 \) entirely into the \( b'/b = 01, 10 \) subspace. The two central swap pulses then apply a phase factor of \(-1\) to any state in this subspace, and so after applying \( V^{-1} \) the net effect of the full sequence will be to multiply the \( c = 3/2 \) state by \(-1\). The fact that \( R \) maps the \( c = 3/2 \) state onto itself immediately implies that \( R \) also maps the \( c = 1/2 \) subspace onto itself, and thus leads to no leakage of the target qubit. Furthermore, since the trace of \( U_{12}(1)U_{34}(1) \) in the \( d = 1 \) sector is \(-1\) (see Eq. (2.59)), the trace of the full sequence \( VU_{12}(1)U_{34}(1)V^{-1} \) in this sector is also \(-1\). Thus, since the \( c = 3/2 \) matrix element of the full sequence is \(-1\), the trace of the operation acting on the \( c = 1/2 \) subspace must be \(0\). Finally, because the two swap pulses \( U_{12}(1)U_{34}(1) \) square to the identity the full sequence for \( R \) squares to the identity. The operation carried out by this sequence on the \( c = 1/2 \) subspace in the \( d = 1 \) sector must therefore also square to the identity and, because it is traceless, it must have the form \( M = \hat{n} \cdot \sigma \).

The set of pulse sequences \( V \) that satisfy Eq. (2.58) defines an infinite class of sequences resulting in two-qubit gates locally equivalent to CNOT. We now show that the fewest number of pulses needed to satisfy the constraint (2.58) is two and for this optimal case the resulting two-qubit gate sequence is the Fong-Wandzura sequence. Without loss of generality\(^7\) we take \( V = U_{23}(t_2)U_{12}(t_1) \) for which,

\[
\langle((\bullet)_{11}((\bullet)_{11})|U_{23}(t_2)U_{12}(t_1)|(\bullet(\bullet\bullet)_3/2)_{11}) = \alpha + \beta e^{-i\pi t_1} + \gamma e^{-i\pi t_2} + \delta e^{-i\pi (t_1+t_2)}.
\] (2.60)

While the values of \( t_1 \) and \( t_2 \) for which \( V \) satisfies Eq. (2.58) can be found by brute force calculation, here we give a simple “pen and paper” procedure.

First consider Eq. (2.60) for the four cases \( t_1 t_2 = 00, 01, 10, \) and \( 11 \). For the trivial case \( t_1 t_2 = 00 \) the matrix element (2.60) is simply the overlap \( F \equiv \langle((\bullet)_{11}((\bullet)_{11})|((\bullet)\quad (\bullet)\quad (\bullet)_3/2)_{11}). \)\(^8\) Next consider

\(^7\)Using any \( V = U_{ki}(t_2)U_{ij}(t_1) \) in our construction for which \([U_{ij}(t_1), U_{kl}(t_2)] \neq 0, (\bullet(\bullet\bullet)_{3/2})_{11} \) is not an eigenstate of \( U_{ij}(t_1), \) and \((\bullet)_{11}(\bullet)_{11} \) is not an eigenstates of \( U_{ki}(t_2), \) yields a two-qubit sequence equivalent to that obtained for the choice made in the text. All other choices are equivalent to sequences with fewer than two pulses, i.e. the case above with \( t_1 = 0 \) or \( t_2 = 0. \)

\(^8\)It is crucial that \( F \neq 0, \) but the actual value of \( F \) is otherwise not needed for our construction. However, it is easily found by direct calculation to be \(1/\sqrt{3}, \) up to a phase factor which is equal to \(1\) for the Condon-Shortley phase convention.

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the cases $t_1t_2 = 01$ and 10, both of which have a single swap pulse. This pulse can be applied directly to the left (for $t_1t_2 = 01$) or right (for $t_1t_2 = 10$) four-spin state in Fig. 2.21(a). Since each swap pulse then acts on a pair of spins with total spin 1 the result is an overall $-1$ using the phase convention of Eq. (2.55). Thus in both cases the matrix element Eq. (2.60) is equal to $-F$.

The only non-trivial case is $t_1t_2 = 11$ for which both pulses are swap pulses. A method for evaluating Eq. (2.60) in this case is sketched in Fig. 2.21(c). First, a pair of swap pulses which combine to the identity, $U_{24}(1)U_{24}(1) = 1$, is inserted at the start of the sequence. We then view the four swap pulses as physical particle exchanges. It is irrelevant that the effect of particle exchange differs from that of a swap pulse by a factor of $-1$ because there are an even number of swap pulses. Applying one of the exchanges acting on spins 2 and 4 to the state $\left(\bullet\bullet\bullet\bullet\right)_{1/2}^1$ then gives a factor +1, since the two spins being exchanged have total spin 1. The remaining three exchanges can then be applied to the state $\left(\bullet\bullet\bullet\bullet\right)_{1/2}^1$ where, referring to the Fig. 2.21(c), they result in a permutation which exchanges the bottom two spins (red oval) with the top two spins (black oval). The net effect is therefore to exchange two spin-1 objects with total spin 1 and, as a result, the right state acquires a factor of $-1$. Thus the $t_1t_2 = 11$ matrix element Eq. (2.60) is equal to $-F$.

Having evaluated the left-hand side of Eq. (2.60) for the four cases $t_1t_2 = 00, 01, 10, \text{ and } 11$, the coefficients appearing on the right-hand side are easily found to be $-\alpha = \beta = \gamma = \delta = F/2$. For these coefficients there are only two solutions which satisfy Eq. (2.58), $t_1t_2 = \frac{3}{2}, \frac{1}{2}$. Figure 2.21(d) shows the resulting sequence for the first solution, which consists of one $\sqrt{\text{SWAP}}$ ($t = \frac{1}{2}$) and one inverse $\sqrt{\text{SWAP}}$ ($t = \frac{3}{2}$) pulse.

### 2.5.3 Explicit Pulse Sequence

Now that we have identified the shortest explicit pulse sequence for an $R$ operation, we can go back to the pulse sequence of Fig. 2.20(d) which, as discussed in Sec. 2.5.1, when applied to a pair of three-spin qubits carries out a controlled-$\left(\hat{n} \cdot \sigma\right)$ gate. This fact is illustrated in Fig. 2.22(a).

Figure 2.22(b) then shows the pulse sequence obtained by inserting the sequence for $V$ from Fig. 2.21(d) into Fig. 2.21(b) and inserting the resulting sequence for $R$ into Fig. 2.22(a). This sequence can be applied to a linear array of spins with nearest-neighbor pulses, and in that case consists of eight swap pulses, six $\sqrt{\text{SWAP}}$ pulses, and six inverse $\sqrt{\text{SWAP}}$ pulses.\footnote{The value of $\hat{n}$ depends on $V$. For the sequence in Fig. 2.21(d) direct calculation gives $\hat{n} = (0, \sqrt{3}/2, -1/2)$ with the direction of the $xy$ component fixed by the Condon-Shortley convention.} After the single-
Figure 2.22: (a) Class of pulse sequences of Fig. 2.20(d) acting on two encoded qubits resulting in a leakage-free controlled-($\hat{n} \cdot \sigma$) gate. (b) Also shown is the full explicit sequence obtained by first inserting the optimal sequence for $V$ from Fig. 2.21(d) into the sequence for $R$ from Fig. 2.21(b) and inserting the result into the sequence from (a). This sequence is equivalent to the Fong-Wandzura sequence.

Qubit rotations are removed, the core Fong-Wandzura sequence as published in Ref. [101] consists of six SWAP pulses, three $\sqrt{\text{SWAP}}$ pulses, and nine inverse $\sqrt{\text{SWAP}}$ pulses. Our sequence can be converted into the Fong-Wandzura sequence through a series of elementary manipulations in which pairs of SWAP pulses are inserted (as in Fig. 2.21(c)) or removed from the sequence, and single SWAP pulses are pulled past other pulses and in some cases combined with $\sqrt{\text{SWAP}}$ pulses to form inverse $\sqrt{\text{SWAP}}$ pulses (and vice versa). The same manipulations can be used to produce sequences applicable to spin geometries other than linear [113]. These manipulations preserve the parity of the sum of the number of SWAP and $\sqrt{\text{SWAP}}$ pulses which is odd for the Fong-Wandzura sequence and even for our construction. This difference in parity is consistent with the fact that a single-qubit operation corresponding to a single SWAP pulse must be added to the core Fong-Wandzura sequence to produce a controlled-(\(\hat{n} \cdot \sigma\)) gate.

2.6 Conclusions

Section 2.3 presents an analytic construction of pulse sequences for exchange-only quantum computation which carry out entangling, leakage-free two-qubit gates on qubits encoded using
three spin-1/2 particles. The resulting pulse sequences, while far from the most efficient, have the unique property that they can be understood in simple geometric terms despite the enormous size of the space of unitary operators acting on the full Hilbert space of the six spin-1/2 particles needed to encode two qubits. The essential idea behind our construction is that this Hilbert space can be built up, spin-by-spin, in such a way that at each level — from two spins, to three, then four, and finally five spins — we are able to reduce the relevant effective Hilbert spaces to either trivial one-dimensional sectors or two-dimensional sectors which can be visualized in the language of spin-1/2 pseudospins.

Because each level of our construction can be understood in terms of effective spin-1/2 pseudospins we are able to work out the required pulse sequences analytically, without having to resort to numerical minimization of a cost function (as in Ref. [46]), the use of genetic algorithms (as in Ref. [101]), or any other numerical method. In addition, because our construction is analytic it allows us to envision alternate pulse sequences for carrying out two-qubit gates, some of which are discussed in Ref. [115]. We believe this general approach of iteratively constructing pulse sequences acting on large Hilbert spaces by effectively reducing the size of the Hilbert space at each level of iteration may have wider applicability for constructing useful pulse sequences for quantum computation.

Section 2.4 then presents an analytic construction which is, to a large degree, parallel to that of the previous section. In fact, the basic operations used in this construction are taken from Sec. 2.3, and the only difference is the choice of spins that we apply these operations to. As a result, we were able to derive a family of 25-pulse sequences that can be used to enact the same entangling two-qubit gates as the 39-pulse sequence derived in the previous section, that is, a controlled-phase gate which multiplies two-qubit states 00, 01 and 10 by the identity and multiplies the 11 state by a phase factor (see also Sec. 1.2.2) which can be arbitrarily chosen.

In Sec. 2.5, we have analytically constructed a class of pulse sequences for carrying out two-qubit gates for exchange-only quantum computation. These sequences can be viewed as elevated versions of the simple three-spin sequences shown in Fig. 2.20(b) which consist entirely of SWAP operations. To carry out this elevation we introduced the four-spin sequence $R$ which is itself built out of a smaller sequence $V$ which satisfies the constraint (2.58). When the shortest pulse sequence
for $V$ is plugged back into the full two-qubit sequence the result is equivalent to the Fong-Wandzura sequence.
CHAPTER 3

GENERATING TWO-QUBIT BRAIDS FOR
TOPOLOGICAL QUANTUM COMPUTATION

3.1 Introduction to Topological Quantum Computation

As discussed in Chapter 1, in a topological quantum computer qubits can be encoded using non-Abelian anyons, such as Fibonacci anyons. Quantum gates are then implemented by moving anyons around one another, a process that can be understood as braiding the (2+1)-dimensional worldlines of anyons around one another. We have introduced the notion of an anyon braid in Sec. 1.3.2, where we also motivated the fact that quantum gates carried out by these braids are robust against local perturbations. Accordingly, topological quantum computation has an inbuilt redundancy against quantum errors.

To use Fibonacci anyons for quantum computation it is natural to encode logical qubits using three or four anyons with fixed topological charge \[53\]. For the qubit encodings of Ref. \[53\], single-qubit gates can be carried out by Fibonacci braiding three anyons within a qubit. Braids which approximate any desired single-qubit gate can be found by carrying out brute force searches over three-anyon braids of some depth, after which either the Solovay-Kitaev method \[118\], used in Refs. \[58, 116\], or the hashing technique based on finding braids that approximate the generators of the icosahedral group of Refs. \[119, 120\] (see also Ref. \[121\]), can be used to systematically improve the braid, with the braid length \(L\) growing as \(L \sim \log \frac{c}{\epsilon}\) with decreasing error \(\epsilon\), where \(c \simeq 4\) for the Solovay-Kitaev method used in Refs. \[58, 122\] and there is evidence that \(c = 2\) for the method of Refs. \[119, 120\]. More recently, using ideas from algebraic number theory, a numerical procedure for finding braids which are asymptotically optimal, i.e. for which the braid length grows as \(L \sim \log \frac{1}{\epsilon}\), has been developed \[123\].

For two-qubit gates, leakage out of the computational space will occur whenever an anyon is braided outside of its home qubit. It is then a nontrivial problem to find braids which suppress this leakage while at the same time perform entangling two-qubit gates. Fortunately, the problem of finding such braids for the six or eight anyons associated with two encoded qubits can be reduced
to that of finding a finite number of three-anyon braids, where a strand can correspond to a single Fibonacci anyon, or a collection of anyons braided as a composite whole [58, 116, 122, 124, 125]. This reduces two-qubit gate construction to a finite number of effective single-qubit gate constructions, which can be carried out using the methods described above.

Reichardt [102] has shown that the braiding properties of Fibonacci anyons allow for an elegant iterative construction of three-anyon braids that carry out purely diagonal operations in certain natural bases. Reichardt used these constructions to present a systematic procedure for distilling Fibonacci anyons from a collection of particles that could be either Fibonacci anyons or topologically trivial particles (an earlier distillation method based on brute force search was presented in Ref. [126]). In the following, we show that constructions closely related to those of Ref. [102] can be used to systematically find braids for carrying out two-qubit gates which become leakage free in the limit of infinite braid length. The convergence of these braids is better than either those found by Solovay-Kitaev [58, 116] or the icosahedral group hashing technique of Refs. [119, 120], and is of the same order as the asymptotically optimal braids found using the procedure of Ref. [123].

The remainder of this chapter, in which we present our work of Ref. [99], is organized as follows. In Sec. 3.2 we review the basic properties of Fibonacci anyons and describe how to encode a logical qubit using either three or four anyons. In Sec. 3.3 we review those aspects of Reichardt’s iterative procedure which are needed to understand our two-qubit gate constructions. Section 3.4 shows how braids generated by this procedure can be used in the two-qubit braid construction of Ref. [122] for four-anyon qubits. Section 3.5 then presents an alternate approach, closely related to that of Ref. [124], which uses these braids to construct two-qubit braids for either three- or four-anyon qubits, as well as outlining how they can be used directly in the four-anyon qubit construction of Ref. [124]. Finally, Sec. 3.6 presents our conclusions.

### 3.2 Computing with Fibonacci Anyons

In the Fibonacci anyon theory [53, 127], there are two possible topological charges: the trivial charge of the vacuum, 0, and the charge of a single Fibonacci anyon, 1. The only nontrivial fusion rule is $1 \times 1 = 0 + 1$, meaning that two objects (where an object can be a single anyon or a collection of anyons) with topological charge 1 can have a total topological charge of either 0 or 1. The other fusion rules follow from the fact that 0 is the trivial charge: $0 \times 0 = 0$, $0 \times 1 = 1 \times 0 = 1$. One
consequence of these fusion rules is that the Hilbert space degeneracy of \( N \) Fibonacci anyons with total topological charge 0 is given by the \((N - 1)\)st Fibonacci number.

In addition to the fusion rules, the essential data needed to compute the unitary operations produced by braiding Fibonacci anyons is contained in two \( 2 \times 2 \) matrices, \( R \) and \( F \).

The \( R \) matrix for Fibonacci anyons is

\[
R = \begin{pmatrix}
  e^{-i4\pi/5} & 0 \\
  0 & e^{i3\pi/5}
\end{pmatrix}.
\]  

(3.1)

This matrix gives the phase factors produced by moving two Fibonacci anyons around one another as shown in the following fusion tree diagram,

\[
\begin{tikzpicture}
  \node (b) at (0,0) {\text{b}};
  \draw (b) edge[->, bend left] (0,1) edge[->, bend right] (0,-1);
\end{tikzpicture}
\]

\[
\begin{tikzpicture}
  \node (b) at (0,0) {\text{b}};
  \draw (b) edge[->, bend left] (0,1) edge[->, bend right] (0,-1);
\end{tikzpicture} = R_{bb}
\]

(3.2)

Here the unlabeled thin lines all carry charge 1, while the labeled thick lines can carry either charge 0 or 1. The above diagram shows that if two Fibonacci anyons are interchanged once with a particular sense, their wavefunction acquires a phase factor of \( e^{-i4\pi/5} \) if their total topological charge (labeled \( b \) in the diagram) is 0, and \( e^{i3\pi/5} \) if their total topological charge is 1. If the anyons are exchanged with the opposite sense the phase factors acquired are the complex conjugates of those given above.

The \( F \) matrix for Fibonacci anyons is

\[
F = \begin{pmatrix}
  \phi^{-1} & \phi^{-1/2} \\
  \phi^{-1/2} & -\phi^{-1}
\end{pmatrix}
\]  

where \( \phi = (\sqrt{5} + 1)/2 \) is the golden mean. This matrix describes a change of basis corresponding to different ways of combining the topological charge of three Fibonacci anyons, as depicted in the following fusion tree diagram,

\[
\begin{tikzpicture}
  \node (b) at (0,0) {\text{b}};
  \draw (b) edge[->, bend left] (0,1) edge[->, bend right] (0,-1);
\end{tikzpicture} = \sum_{b' \in \{0,1\}} F_{bb'} \begin{tikzpicture}
  \node (b') at (0,0) {\text{b'}};
  \draw (b') edge[->, bend left] (0,1) edge[->, bend right] (0,-1);
\end{tikzpicture}
\]

(3.4)

where, again, unlabeled thin lines are all assumed to carry the charge 1 and the labeled thick lines can carry either charge 0 or 1.

Figure 3.1(a) shows the 0 and 1 states of a logical qubit encoded using four Fibonacci anyons with total charge 0, using fusion tree diagrams as well as an alternate notation in which ovals enclose collections of particles and are labeled by the total topological charge of the enclosed particles. In the text, we will represent states in the oval notation by replacing ovals with parentheses. The
qubit states shown in Fig. 3.1(a) are then \( |0_L\rangle = ((\bullet)_{0}(\bullet)_{0})_0 \) and \( |1_L\rangle = ((\bullet)_{1}(\bullet)_{1})_0 \) where \( \bullet \) denotes a Fibonacci anyon. A similar qubit encoding using three anyons with total charge 1 is shown in Fig. 3.1(b).

Single-qubit operations are carried out by braiding Fibonacci anyons within a given qubit. The unitary operation produced by such a braid can always be determined using the \( R \) and \( F \) matrices. Braiding objects within a given collection of objects will not change the total topological charge of the collection, and so there is no danger of leakage errors out of the encoded qubit space when carrying out such single-qubit gates. Braids which carry out a desired single-qubit operation can be found by a combination of brute force search over braids up to a given length and the Solovay-Kitaev method [118, 58, 116], as well as other numerical methods [119, 120, 123].

Finding braids for two-qubit gates is more difficult. When anyons from two distinct qubits are braided, there will inevitably be leakage out of the encoded qubit space. Note that any two-qubit braid that enacts an operation on a pair of three-anyon qubits [Fig. 3.1(b)] will enact the same operation on a pair of four-anyon qubits [Fig. 3.1(a)]. This is because a three-anyon qubit, which has total charge 1, is equivalent to a four-anyon qubit, which has total charge 0, with one anyon removed, i.e. \( ((\bullet)_{a}(\bullet)_{a})_0 = ((\bullet)_{a}(\bullet)_{a})_0 \) with \( a = 0 \) or 1.

### 3.3 Reichardt Sequence and Weaving

The following observation due to Reichardt [102] plays a central role in our systematic two-qubit gate constructions. Starting with any unitary \( 2 \times 2 \) matrix, \( U_0 \), after each iteration of the equation

\[
U_{k+1} = U_k R U_k^\dagger R^3 U_k R^3 U_k^\dagger R U_k,
\]  

(3.5)
the magnitude $x_k$ of the off-diagonal matrix elements of $U_k$ is greatly reduced (provided $x_k \neq 1$), with

$$x_{k+1} = x_k^5.$$  \hfill (3.6)

This reduction is due to the geometric fact that the sequence of operations (3.5) when viewed as rotations automatically cancels up to 4th order any deviations $U_k$ may have from being a pure $z$-axis rotation [128].

Our two-qubit gates are built out of braids that are constructed iteratively using (3.5). We focus on weaves — as described in Sec. 1.3.2, braids in which only one particle (or object), the weft, is mobile while the other particles, the warp, remain fixed. It has been shown that any unitary operation that can be carried out by braiding can be carried out by weaving [129].

To construct these weaves we follow a procedure similar to that used by Reichardt [102]. We begin by setting $U_0$ equal to a “seed” product of $R$ and $F$ matrices which has the form

$$FR^{n_2}FR^{n_1-1} \cdots FR^{n_2}F.$$  \hfill (3.7)

Iterating (3.5) will then result in a sequence of matrices, $U_k$, which become diagonal in the $k \to \infty$ limit. Each $U_k$ in this sequence will also be expressed as a matrix product of the form (3.7).

To convert products of $F$ and $R$ matrices into weaves we use the hexagon diagram shown in Fig. 3.2(a). The fusion diagrams, labeled 1 through 6, at the vertices of this hexagon are given in two different bases, $\bigtriangledown$ and $\bigtriangledown$, and we refer to $\bigtriangledown$ as the standard basis. The matrix operations $U_k$ of all weaves that we use to construct two-qubit gates will become diagonal in this standard basis.

For example, let us turn the product $FR^3FR^{-2}FRF$ into a weave. As will always be the case in what follows, we start at fusion diagram 1, circled in the upper left corner of Fig. 3.2(a), and weave the weft, denoted $\bigstar$, around the two warp particles, each denoted $\bullet$. The first (rightmost) matrix in our example product is $F$. Applying $F$ moves us one step around the hexagon in a counterclockwise sense to diagram 2, resulting in a basis change. Next we apply $R$, which takes us one more counterclockwise step around the hexagon to diagram 3 by weaving the weft once around

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1Here the usage of the terms “weft” and “warp” is opposite to that of Ref. [129] but equivalent to that of Ref. [116]. We choose to be consistent with Ref. [116] because for this choice the meaning of these terms are closest to their meaning in the context of ordinary weaving.
the central warp. This is followed by another $F$ which takes us yet one more counterclockwise step around the hexagon to diagram 4, resulting in another basis change. Next we apply $R^{-2}$, and, in this case, because there are an even number of $R$ operations, the weft weaves around the rightmost warp twice (with the opposite sense of the initial $R$ operation) and we return to diagram 4. Thus, rather than progressing around the hexagon, after applying $R^{-2}$ (and whenever there are an even number of $R$ operations) we remain at the same fusion diagram. The next $F$ then takes us one step around the hexagon in a clockwise sense to diagram 3, resulting in a basis change. This is followed by $R^3$, and because the weft now weaves three times around the leftmost warp it does not return to its original position; thus we move one more clockwise step around the hexagon to diagram 2. The final $F$ operation returns us to the original fusion diagram 1 from which we began. The resulting weave, shown in Fig. 3.2(b), carries out the operation $FR^3FR^{-2}FRF$ in the standard basis.
As a second example, consider the product $FR^5F$. Following the same procedure as above, the first operation $F$, then $R^5$, and finally $F$ again will move us one counterclockwise step each around the hexagon to diagram 4, circled in the lower right corner of Fig. 3.2(a). As shown in Fig. 3.2(c), in this process we have woven $\ast$ five times around the central warp.

The two weaves discussed above are examples of the two kinds of weaves we use to construct braids for two-qubit gates. When turning a product of $F$ and $R$ matrices into a weave, we progress around the hexagon in Fig. 3.2(a) starting from the circled diagram 1. For the first kind of weaves, which we call phase weaves, the final diagram is the same as the starting diagram, and the weft returns to its original position [see Fig. 3.2(b)]. For weaves of the second kind, which we call exchange weaves, the final diagram is the circled diagram 4 and the weft exchanges its position with the central warp [see Fig. 3.2(c)].

For the first two examples, we could have constructed the corresponding weaves by noting that in the standard basis $R$ and $FRF$ are the elementary braid matrices for interchanging the two rightmost particles and the two leftmost particles, respectively. However, if we followed the above procedure for the product $FRFR^{-1}F$ we would have gone nearly all the way around the hexagon of Fig. 3.2(a), ending at fusion diagram 6. This diagram is not in the standard basis, and so we need to perform an additional odd number of $R$ operations to return to diagram 1. Since our goal is to produce weaves that carry out diagonal operations in the standard basis, and $R$ itself is diagonal in this basis, we are always free in our constructions to multiply any product of the form (3.7) on the right or left by any power of $R$. The supplemented sequence $RFRFR^{-1}F$ then takes us back to the starting diagram 1. Note that this last operation is denoted $R'$ in Fig. 3.2(a). We use this notation to distinguish this operation from $R$ because it is based on the weave represented by the following fusion tree diagram,

$$
\begin{array}{c}
\begin{array}{c}
\bullet
\end{array}
\rightarrow
\begin{array}{c}
\begin{array}{c}
\circ
\end{array}
\end{array}
= R'_{bb}.
\end{array}
$$

(3.8)

Here

$$
R' = \begin{pmatrix}
1 & 0 \\
0 & e^{-i\pi/5}
\end{pmatrix} = e^{i4\pi/5}R,
$$

(3.9)

thus $R$ is equal to $R'$ up to an overall phase and so can be used when iterating (3.5). Note that the sense used to define the $R'$ exchange is the opposite of that used to define $R$, and that after carrying out an odd number of $R'$ operations there will also be an associated change of basis. The phase weave which results for this third example sequence, $RFRFR^{-1}F$, is shown in Fig. 3.2(d).
Similarly, matrix products of the form (3.7) with final diagrams 2, 3 or 5 can be turned into exchange weaves by multiplying odd numbers of $R$ matrices on the left and/or right. Specifically, if the final diagram is 2 or 3 we multiply by an odd number of $R$ operations from the right and so start progressing around the hexagon in a clockwise rather than counterclockwise sense. Due to the symmetry of the hexagon, the new final diagram will then be either 4 or 5. Furthermore, any product of $F$ and $R$ matrices with final diagram 5 needs to be multiplied by an odd number of $R$ operations from the left in order to proceed to diagram 4. In what follows we always choose the power of the additional $R$ operations to minimize the total number of elementary interchanges of the weave.

Our last example is the operation $F$. In the hexagon, this simply takes us one counterclockwise step from diagram 1 to 2. Multiplication by one $R$ operation on each side results in the product $RFR$ which takes us three clockwise steps around the hexagon from diagram 1 to 4. Figure 3.2(e) shows the corresponding exchange weave.

We have thus established how to generate three-anyon weaves that carry out operations whose matrix representations become diagonal in the standard basis. Starting with a seed $U_0$ of the form (3.7) and iterating (3.5) results in a sequence of matrices $U_k$ which converges quickly to diagonal form. As described above, we can turn every $U_k$, given as a product (3.7), into a weave using Fig. 3.2(a). In this process one moves around the hexagon, starting at fusion diagram 1. If the final diagram for a given $U_0$ is diagram 1 or 6 we refer to the corresponding matrix product (3.7) as a phase seed, and every resulting operation $U_k$ can be used as a phase weave. Any other $U_0$ will be referred to as an exchange seed for which all resulting operations $U_k$ can be used as exchange weaves.

The leakage error of the two-qubit braids constructed below is proportional to the size of the off-diagonal elements $x_k$ of the matrix representation of the operation $U_k$ in the standard basis. Given (3.6), and the fact that the weave length grows by a factor of 5 with each iteration of (3.5) (not counting the constant number of additional elementary weaves due to the $R$ operations which appear explicitly) we see that the length, $L$, of the weave grows as $L \sim \log \frac{1}{x}$ [102], which is significantly better than the polylogarithmic growth that occurs when using the Solovay-Kitaev method [118] and is comparable to the optimal case achieved using the number-theoretic based methods of Ref. [123].
A potential drawback to using the iterative approach described here is that, because the braid length grows exponentially with the number of iterations of (3.5), it is possible to significantly overshoot the desired braid length dictated by a given required gate accuracy. A similar issue arises in the standard Solovay-Kitaev approach [118], but is not present for the number-theoretic approach of Ref. [123]. We envision that in a practical implementation this issue can be addressed by first forming a library of exchange or phase seeds of minimum off-diagonal matrix elements (in the standard basis) for each given length up to some finite length, e.g. by brute force search. Then, given this library, one can choose seeds of the appropriate length so that iterating (3.5) a finite number of times will generate a weave of approximately the desired length without danger of significant overshoot.

### 3.4 Controlled-Phase Gates

In this section we show how the phase weaves of the previous section can be used to directly carry out entangling two-qubit gates for four-anyon qubits using a construction presented in Ref. [122].

In Fig. 3.3(a), the box labeled $U_k$ with three incoming and outgoing anyon strands represents a generic phase weave which returns the weft, ⚫, to its original position. As described in the previous section, this weave is obtained by iterating (3.5) starting from a phase seed $U_0$. The matrix $U_k$ corresponding to the operation carried out by this weave quickly converges to a diagonal matrix, so to a good approximation its action for large $k$ is to multiply the state $(\bigstar(\bullet\bullet)_0)_1$ by a phase factor of $e^{i\theta_k}$. As shown in the figure, in the $k \to \infty$ limit this approximation becomes exact and the phase $\theta_k$ converges to a limiting value $\theta_\infty$. The convergence behavior of $\theta_k$ is discussed below.
Following Hormozi et al. \cite{122}, any phase weave can be used to construct a two-qubit gate. Figure 3.3(b) shows two four-anyon qubits in states $a$ and $b$ and a braiding pattern for the bottommost six anyons. To construct this pattern, neighboring pairs of anyons are first grouped into three objects, one with total charge $a$ in the upper qubit and two with total charge $b$ in the lower qubit, as indicated in the figure. The three-anyon weave shown in Fig. 3.3(a) is then carried out as a “superweave” with the charge $a$ object as the weft and the two charge $b$ objects as the warp.

The two-qubit gate character of the resulting operation becomes evident when considering different two-qubit states defined by $a$ and $b$. Note that any anyon weave that returns the weft to its original position results in the identity operation if either the weft or each warp object has charge zero. The operation $U_k$ thus trivially enacts the identity if $a = 0$ or $b = 0$. In the nontrivial case $ab = 11$ the superweave carries out the phase weave of Fig. 3.3(a) and for $k \to \infty$ applies the phase factor $e^{i\theta_k \delta \theta}$. As shown in Fig. 3.3(b), the two-qubit braid thus enacts a controlled-phase gate which for nontrivial phases $\theta_k \neq 0$ (mod $2\pi$) is entangling.

Figure 3.4(a) shows an example phase weave corresponding to the seed $FR^4F$. The weaves that belong to the first and second iterations of (3.5) are shown in Figs. 3.4(b) and (c). Recall that when turning such sequences into weaves, some $R$ operations are realized as $R'$, which is equal to $R$ up to an overall phase. For the current construction we need to keep track of this overall phase because the value of $\theta_k$ determines the two-qubit gate of Fig. 3.3. In Figs. 3.4(b) and (c) we see that all $R$ operations which appear explicitly in (3.5) are $R'$ operations. This is always the case for phase weaves so that in the present section the iteration prescription can unambiguously be written as

\begin{equation}
U_{k+1} = U_k R'^\pm 1 U_k^\dagger R'^\pm 3 U_k R'^\pm 3 U_k^\dagger R'^\pm 3 U_k^\dagger R'^\pm 1 U_k, \tag{3.10}
\end{equation}

provided the starting operation $U_0$ is that obtained by turning the phase seed into a weave following Sec. 3.3. Note that in (3.10) we have used the fact that the sign of the powers of $R$ in (3.5) can be changed without altering the result (3.6).

Denoting the two states in the standard basis $\bigotimes$ with total charge 0 or 1 of the two rightmost anyons by $|0\rangle$ or $|1\rangle$, respectively, and letting

\begin{equation}
x_k = |\langle 1|U_k|0\rangle|, \quad \theta_k = \arg \langle 0|U_k|0\rangle, \tag{3.11}
\end{equation}

direct calculation yields

\begin{equation}
x_{k+1} = x_k^5, \quad \theta_{k+1} = \theta_k + s_k \delta \theta(x_k), \tag{3.12}
\end{equation}

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Figure 3.4: (a) Weave corresponding to phase seed $FR^4F$. (b) Weave obtained with this seed after one iteration of (3.10). (c) Weave obtained with this seed after a second iteration of (3.10). In (b) and (c) dashed lines divide parts of the weave corresponding to $U_k$ and $U_k^\dagger$ from those corresponding to the $R'$ and $R'^3$ operations appearing explicitly in (3.10). For the seed $FR^4F$ the magnitude of the initial off-diagonal matrix elements is $x_0 \simeq 0.571$ and the initial phase is $\theta_0 \simeq 0.546\pi$. After two iterations $x_2 \simeq 8.30 \times 10^{-7}$ and $\theta_2 \simeq 0.488\pi$.

(d) $\delta\theta$, shift in the phase of $\langle 0|U|1 \rangle$ after one iteration of (3.10), plotted as a function of $x = |\langle 1|U|0 \rangle|$, as well as $\Delta\theta^+, \Delta\theta^-$, and $\Delta\theta^\pm$ corresponding to different choices for the signs $s_k$ in (3.15). (e) Controlled-phase gate (see Fig. 3.3(b)) with $\theta_2 \simeq \theta_\infty \simeq 0.488\pi$ obtained using the second iteration phase weave shown in (c).

where

$$\delta\theta(x) = -\arcsin\left(\frac{5^{1/4}(\phi^{-3/2}x^2 + \phi^{1/2}x^4)}{2\sqrt{1 + x^2 + x^4 + x^6 + x^8}}\right). \quad (3.13)$$

Here the sign $s_k = \pm 1$ in (3.12) is equal to the sign of the powers of $R'$ in (3.10).

For the $k \to \infty$ phase we then have

$$\theta_\infty = \theta_0 + \Delta\theta(x_0), \quad (3.14)$$

where

$$\Delta\theta(x_0) = \sum_{k=0}^{\infty} s_k \delta\theta(x_0)^{5^k}. \quad (3.15)$$

The function $\delta\theta(x)/\pi$ is shown in Fig. 3.4(d). As $x \to 0$, $\delta\theta(x)$ vanishes quadratically, and as $x \to 1$, $\delta\theta(x) \to \pi/5$. Three different results for $\Delta\theta(x)$, corresponding to different choices for the
Table 3.1: Example phase seeds.

<table>
<thead>
<tr>
<th>Seed</th>
<th>$x_0$</th>
<th>$\theta_0/\pi$</th>
<th>$(\theta_0 + \Delta\theta^+)/\pi$</th>
<th>$(\theta_0 - \Delta\theta^+)/\pi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$FR^2F$</td>
<td>0.924</td>
<td>1</td>
<td>0.737</td>
<td>-0.737</td>
</tr>
<tr>
<td>$FRFR^3F$</td>
<td>0.924</td>
<td>1</td>
<td>0.737</td>
<td>-0.737</td>
</tr>
<tr>
<td>$FR^3FR^{-3}F$</td>
<td>0.882</td>
<td>0</td>
<td>-0.207</td>
<td>0.207</td>
</tr>
<tr>
<td>$FR^4F$</td>
<td>0.571</td>
<td>0.546</td>
<td>0.488</td>
<td>0.604</td>
</tr>
<tr>
<td>$FR^5FR^5F$</td>
<td>0.415</td>
<td>1</td>
<td>0.997</td>
<td>-0.997</td>
</tr>
<tr>
<td>$FRFRF$</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

sequence of signs, $\{s_k\}$, are also shown in Fig. 3.4(d). $\Delta\theta^+$ corresponds to choosing $s_k = +1$ for all $k$, $\Delta\theta^-$ corresponds to choosing $s_0 = +1$ and $s_k = -1$ for all $k > 0$, and $\Delta\theta^\pm$ corresponds to choosing $s_k = (-1)^k$ for all $k$. The Taylor expansions of all these functions agree up to 8th order in $x$ and only begin to noticeably deviate from one another for $x$ larger than $\sim 0.6$. As a consequence, for seeds with small $x_0$ (which are desirable since they will converge faster to diagonal matrices), only the first contribution to the phase, $\delta\theta(x_0)$, will be appreciable, with $\theta_\infty \simeq \theta_0 \pm \delta\theta(x_0)$.

Figure 3.4(e) shows an explicit example two-qubit braid based on the weave of Fig. 3.4(c). Note that in Fig. 3.4(e), we have eliminated trivial sequences of braids whenever one interchange is directly followed by its inverse. In addition, using the fact that $R^{10} = 1$, we reduce the number of consecutive windings experience by neighboring strands to be less than or equal to five.

Table 3.1 lists example phase seeds together with their $x_0$ and $\theta_0$ values. Given a nontrivial phase weave (i.e. one for which $\theta_\infty \neq 0 \mod 2\pi$) one can always, as above, construct a leakage-free entangling two-qubit gate. The first two entries with identical values show that different seeds can be effectively equivalent. The last entry of Table 3.1, $FRFRF$, results in a weave that carries out a trivial operation for which $\theta_k = 0$ for all $k$ and is thus not useful in our two-qubit gate construction.

In this section we described two-qubit gates whose specific operation cannot be a priori chosen because it depends on the phase weave used to construct the two-qubit braid. In the next section we present a new construction based on exchange weaves for which the resulting operation of the entangling two-qubit gate is independent of the weave used.

### 3.5 Controlled-Braid Gates

We now show how the exchange weaves of Sec. 3.3 can be used to carry out two-qubit gates. Our approach is similar to that of Xu and Wan [124] where anyons are exchanged between qubits
Figure 3.5: (a) Box representing an exchange weave, which in the $k \to \infty$ limit maps $(\star(\bullet\bullet)_0)_1$ to $(\bullet(\star\bullet)_0)_1$. (b) Controlled-$R^2$ gate construction for two three-anyon qubits.

while essentially preserving the stored quantum information. These exchanges, whose corresponding braids can be found via methods based on brute force search [124], can be performed more efficiently by the exchange weaves introduced in this chapter. One property of the two-qubit braids of Ref. [124] is that they can only be applied to qubits encoded using four anyons each. Here, we construct new two-qubit braids that can be applied to a pair of either three- or four-anyon qubits.

The box labeled $U_k$ shown in Fig. 3.5(a) represents a three-anyon exchange weave that carries out an operation $U_k$ and is obtained, as described in Sec. 3.3, by choosing an exchange seed $U_0$ and iterating (3.5) $k$ times. This exchange weave switches the positions of the weft $\star$ and the central warp, while the matrix representation of $U_k$ in the standard basis converges to diagonal form for large $k$. It follows that acting with $U_k$ on $(\star(\bullet\bullet)_b)_1$, with $b = 0 \text{ or } 1$ in the limit of $k \to \infty$ results in the state $(\bullet(\star\bullet)_b)_1$ up to a phase factor [as indicated by $\hat{=} \text{ below in the text as well as in Fig. 3.5(a)}$] whose value will be shown shortly to be irrelevant.

Figure 3.5(b) shows two three-anyon qubits (given in a convenient basis for what follows) and a braiding pattern for the middle four anyons $((\bullet\bullet)_a(\bullet\bullet)_d)$, where $d = 0 \text{ or } 1$. To construct this pattern, we first group the two anyons with total charge $a$ into a single object. The three-anyon weave shown in Fig. 3.5(a) is then carried out as a superweave with this charge $a$ object as the weft and the two uppermost anyons in the bottom qubit as the warp.

To determine the action of the two-qubit weave of Fig. 3.5(b) first note that by the end of the weave the weft is returned to its original position. It follows that if $a = 0$ this braid carries out the identity operation. In the non-trivial case of $a = 1$ we replace the object $(\bullet\bullet)_{a=1}$ by a single anyon, $\star$,

$$((\bullet\bullet)_{a=1}(\bullet\bullet)_d) \rightarrow (\star(\bullet\bullet)_d). \quad (3.16)$$
Table 3.2: Example exchange seeds.

<table>
<thead>
<tr>
<th>Seed</th>
<th>$x_0$</th>
<th>Initial Sense</th>
</tr>
</thead>
<tbody>
<tr>
<td>$FR^3F$</td>
<td>0.972</td>
<td>◯</td>
</tr>
<tr>
<td>$F$</td>
<td>$\phi^{-1/2} = 0.786$</td>
<td>◯</td>
</tr>
<tr>
<td>$FRF$</td>
<td>$\phi^{-1/2} = 0.786$</td>
<td>◯</td>
</tr>
<tr>
<td>$FRFR^2F$</td>
<td>$\phi^{-1/2} = 0.786$</td>
<td>◯</td>
</tr>
<tr>
<td>$FR^3F$</td>
<td>0.300</td>
<td>◯</td>
</tr>
<tr>
<td>$FR^3FR^5FR^3F$</td>
<td>0.0438</td>
<td>◯</td>
</tr>
</tbody>
</table>

In the limit of $k \to \infty$ the first operation shown in Fig. 3.5(b), $U_k$, then carries out the mapping

$$
\lim_{k \to \infty} U_k(\star(\bullet\bullet)_b)_d \cong (\bullet(\star\bullet)_b)_d. \tag{3.17}
$$

up to a phase factor that depends on both quantum numbers $b$ and $d$. Notice that in the case of $bd = 10$ this map is already exact for any finite $k$, because the Hilbert space of three Fibonacci anyons with total charge 0 is one-dimensional. As shown in the figure, in the next step we weave $\star$ twice around the warp inside the oval with total charge $b$, thus carrying out an $R^2$ operation on the Hilbert space spanned by the states (3.17) with $b = 0$ and 1. Finally, the operation $U_k^\dagger$ exchanges $\star$ with what is now the topmost warp. Importantly, $U_k^\dagger$ further multiplies each state with given quantum numbers $bd$ by the complex conjugate of the phase factor that was applied by $U_k$. Since the $R^2$ operation in the center of the sequence is diagonal in $b$ and $d$ the phase factors of $U$ and $U^\dagger$ cancel one another. The resulting operation carried out by the two-qubit braid of Fig. 3.5(b) is then an $R^2$ operation acted on the qubit in state $b$ if $a = 1$ and the identity if $a = 0$. We thus refer to the weave which carries out the intermediate $R^2$ operation as a controlled braid, and the resulting two-qubit gate as controlled-braid gate where the control (target) qubit is the qubit with state label $a$ ($b$).

When determining the operation carried out by the braid of Fig. 3.5(b) we made use of the crucial property that the quantum number $a$ is conserved. In the middle step of our construction, for $a = 1$ the $R^2$ superweave applied to $((\bullet\bullet)_{a=1}\bullet)_b$ is carried out with $((\bullet\bullet)_{a=1}\bullet)_b$ as the weft object and thus trivially conserves $a$. Note that this $R^2$ operation can be replaced by any $R^n$ operation with $n$ even, yielding a total of four distinct two-qubit gates. However, if we allow for arbitrary controlled braids of these three anyons $((\bullet\bullet)_{a=1}\bullet)_b$ under the constraint that $a$ is conserved, then we uncover an infinite number of two-qubit entangling braids for three-anyon qubits. One natural
Figure 3.6: (a) Weave corresponding to the exchange seed $FR^3F$. (b) Weave obtained with this seed after one iteration of (3.5). (c) Weave obtained with this seed after a second iteration of (3.5). For the seed $FR^3F$ the magnitude of the initial off-diagonal matrix elements is $x_0 \approx 0.300$, and, after two iterations, $x_2 = 8.67 \times 10^{-14}$. In (b) and (c) dashed lines divide parts of the weave which corresponding to $U_k$ and $U_k^\dagger$ from those corresponding to the $R$ and $R^3$ operations appearing explicitly in (3.5). (d) Controlled-$R^2$ gate (see Fig. 3.5(b)) obtained using the second iteration exchange weave shown in (c). The controlled braid which enacts an $R^2$ operation only if the control qubit is the state $1$ is indicated by the dashed box.

choice for these controlled braids are phase weaves $((\bullet\bullet)_a=1 \star)_b \rightarrow e^{i\theta_b}((\bullet\bullet)_a=1 \star)_b$ (to a good approximation) with the rightmost anyon as the weft $\star$ and the two leftmost anyons as the warp. [Note that the $a = 0$ sector gets multiplied by an overall phase factor because here we have $((\bullet\bullet)_a=0 \star)_1 \rightarrow e^{i\theta_{a=0}}((\bullet\bullet)_a=0 \star)_1$.] While the length $L$ of the resulting two-qubit braid then grows as $L \sim \log \frac{1}{x}$, control of the exact two-qubit operation, which depends on the phase factors applied by the controlled weave, is limited (as for the two-qubit braids of the previous section).

We now construct an example exchange weave starting from the seed $FR^3F$. Figures 3.6(a) through (c) show the weaving patterns of the seed as well as the first and second iterations. The sense with which one starts progressing around the hexagon in Fig. 3.2(a) for a given matrix product of the form (3.7) for an exchange weave gets reversed after iterating (3.5). As discussed in Sec. 3.3, whenever this sense is clockwise one needs to multiply the product on the right by an odd number of $R$ operations. For the example, $FR^3F$, the initial sense is counterclockwise and so for the first iteration this sense is clockwise while for the second it is again counterclockwise. We therefore multiply the first iteration by an additional $R$ operation from the right. Since, further, the final diagram of this supplemented product is diagram 5 in the hexagon, we also multiply the sequence by one additional $R$ operation on the left. Both additional $R$ operations are indicated in Fig. 3.6(b).
Figure 3.6(d) shows the explicit two-qubit gate braid of Fig. 3.5 that is obtained when replacing the exchange weaves $U_k$ and $U_k^\dagger$ by the weave of Fig. 3.6(c) and its inverse, respectively. As in the two-qubit phase gate shown in Fig. 3.3(e), all redundant braids have been eliminated and the fact that $R^{10} = 1$ has been used to reduce the number of windings whenever possible.

Table 3.2 lists example exchange seeds together with the magnitude of their off-diagonal elements, $x_0 = |\langle 0 | U_0 | 1 \rangle|$, and the sense with which one starts to move around the hexagon of Fig. 3.2 when turning the seed into a weave. The key parameter of any seed is the absolute value of its off-diagonal matrix elements, $x_0$, which determines how many times (3.5) needs to be iterated to achieve a desired error.

It is instructive to contrast the closely related two-qubit gate construction of Ref. [124] with the one presented above. The braids of Ref. [124] are applied to a pair of four-anyon qubits,

$$(\bullet\bullet\bullet\bullet)_{a=1}(\bullet\bullet\bullet\bullet)_{b=1}.$$  \hfill (3.18)$$

Similar to the controlled-phase gates in Sec. 3.4, as well as the controlled-$R^n$ gates with $n$ even constructed above, braids constructed using the method of Ref. [124] are superweaves in which an anyon pair $(\bullet\bullet)_{a}$ is a weft object that is restored to its original position at the end of the weave. Carrying out these weaves therefore results in the identity operation for $a = 0$ and a nontrivial operation for $a = 1$, i.e., a controlled-operation with the control and target being the qubits with state labels $a$ and $b$, respectively.

We now focus on the case of $a = 1$ and replace the left $(\bullet\bullet)_{a=1}$ pair inside the control qubit in (3.18) by $\star$,

$$(\bullet\bullet\bullet\bullet)_{b}(\bullet\bullet\bullet\bullet)_{a=1}(\bullet\bullet\bullet\bullet)_{a=0} \rightarrow (\bullet\bullet\bullet\bullet)_{b}(\bullet\bullet\bullet\bullet)_{a=0}(\star(\bullet\bullet)_{a=1})_{0}. \hfill (3.19)$$

In the Xu-Wan construction exchange weaves are carried out on the control qubit and the rightmost anyon of the target qubit, $(\bullet(\star(\bullet\bullet)_{a=1})_{0})_{1}$. If we follow the exchange weave construction of Sec. 3.3 to obtain a weave that carries out an operation $U_k$ which for $k \rightarrow \infty$ becomes diagonal in the standard basis, its inverse $U_k^\dagger$ will carry out the operation

$$\lim_{k \rightarrow \infty} U_k^\dagger(\bullet(\star(\bullet\bullet)_{a=1})_{0})_{1} \doteq (\star(\bullet\bullet)_{a=1})_{0}.$$  \hfill (3.20)$$

up to some phase factor, with $\star$ the weft and $\bullet$ and $(\bullet\bullet)_{a=1}$ the warp. It follows that after an application of $U_k^\dagger$ the pair of particles $\star = (\bullet\bullet)_{a}$ is inserted into the target qubit, that now has the
form

\[((\bullet) b (\star) b) 0, \]

(3.21)

without causing leakage because the total charge of the rightmost three anyons in (3.20) is 0.

Following Ref. [124], a two-qubit braid can be constructed by first inserting \(\star\) into the target qubit using \(U_k^\dagger\) as given in (3.20), then carrying out a weave with \(\star\) still the weft that restores it to the rightmost position inside the target qubit as given in (3.21), and finally extracting \(\star\) using \(U_k\) [whose action is given by inverting (3.20)]. Thus, for example, if the intermediate weave is an \(R^2\) weave inside the target qubit, for which \(\star\) is braided once all the way around the anyon to its immediate left in (3.21), the result of the entire two-qubit braid would be to carry out a controlled-\(R^2\) gate.

As opposed to the exchange weave in (3.17) for which different states within the \(a = 1\) sector, \(((\bullet) a = 1 (\bullet) b) d\), are multiplied by different phase factors, the exchange weaves as applied in (3.20) multiply the entire \(a = 1\) two-qubit sector by a single overall phase factor. Accordingly, while the controlled braids used in our three-anyon qubit construction must conserve the quantum numbers \(b\) and \(d\), and hence must be diagonal in \(b\), the controlled operations in the Xu-Wan construction do not need to conserve \(b\), and so are less restricted at the price of using four-anyon qubits.

Finally, as noted by Reichardt [102], because the matrices \(U_k\) obtained by iterating (3.5) become diagonal as \(k \to \infty\), the matrices \(XU_k\) [where \(X = (\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix})\)] become off-diagonal in the same limit at the same optimal rate. This, combined with the fact that \(XR^nX = e^{-in\pi/5}R^{-n}\), implies that for any phase seed with a non-diagonal \(U_0\) in the standard basis, iterating

\[U_{k+1} = U_k R^{-1} U_k^\dagger R^3 U_k R^{-3} U_k^\dagger R U_k,\]

(3.22)

but otherwise following the phase weave construction of Sec. 3.3, will result in a sequence of weaves for which \(U_k\) becomes off-diagonal in the standard basis. These weaves asymptotically carry out \(\pi\) rotations about axes lying in the \(xy\) plane, the direction of which within this plane, like the phase in the controlled-phase gate construction of Sec. 3.4, cannot be directly controlled. Because these weaves return the weft to its original position they can be used as the intermediate controlled braid in the four-anyon qubit Xu-Wan construction [124] reviewed above. The resulting two-qubit braid would then be locally equivalent to a controlled-\(\text{NOT}\) (\(\text{CNOT}\)) gate, regardless of the direction of the rotation axis.
3.6 Conclusions

In this chapter we have shown how to use a construction introduced by Reichardt [102] for distillation of Fibonacci anyons to systematically generate weaving patterns that can be used to carry out two-qubit gates which become leakage free in the limit of infinite braid length. One construction, based on a two-qubit gate construction given in Ref. [122], requires four-anyon qubits. As discussed in Sec. 3.4, the resulting two-qubit gates carried out by these braids are locally equivalent to controlled-rotation gates, for which the rotation angle depends on the seed weave and cannot be freely chosen. A second construction, described in Sec. 3.5, is closely related to that given in Ref. [124], although unlike in that work, our two-qubit gates can be applied to three-anyon qubits as well as four-anyon qubits. This procedure can be used to generate two-qubit braids that carry out controlled-$R^n$ gates, with $n$ even, as well as other controlled $z$-axis rotation gates with similar properties to those of Sec. 3.4. In Sec. 3.5 we also outlined how the original four-anyon qubit construction of Ref. [124] can be carried out using a combination of exchange weaves and weaves obtained in the same fashion as the phase weaves of Sec. 3.3, but with a different iteration equation, also introduced in Ref. [102], with the result converging to a two-qubit gate that is locally equivalent to CNOT.

The constructions presented here yield two-qubit braids that converge efficiently, in the sense that their length grows logarithmically with inverse error, and can be carried out systematically without the need for any numerical search techniques. It is possible that the iteration procedures of Ref. [102] can be used in different two-qubit gate constructions not considered here. Even if this is the case, for universal quantum computation it will of course be necessary to supplement these two-qubit gates with arbitrary single-qubit rotations for which other braid compilation techniques, e.g. either Solovay-Kitaev or the number-theoretic method of Ref.[123], will be necessary.
CHAPTER 4

OUTLOOK

In this final chapter, we summarize our findings presented in Chapters 2 and 3. We further discuss questions and topics related to our work for possible future studies.

4.1 Summary

In this Dissertation we have presented work on the problem of entangling logical qubits, encoded by either spin-1/2 particles or Fibonacci anyons, using two-qubit quantum gates. In the introductory chapter (Sec. 1.3) we explained the fundamental mechanisms for realizing quantum gates in the two computing proposals considered in the main part of this thesis. A joint feature of these proposals is the difficulty of determining precise procedures for carrying out two-qubit gates. Here we have introduced new methods for solving the problem of finding such procedures. As opposed to all prior work, our methods are the first which can be carried out completely analytically and without using any numerical techniques.

In Chapter 2 we focus on exchange-only spin-based quantum computation, in which the only resource for carrying out quantum gates is turning on-and-off, or pulsing, the Heisenberg exchange Hamiltonian $J \mathbf{S}_1 \cdot \mathbf{S}_2$ between spin-1/2 particles. Two-qubit gates are then carried out by long sequences of exchange pulses. Due to the complexity of the problem of obtaining suitable two-qubit pulse sequences, all such pulse sequences that were previously obtained were found by numerical searches over many sequences. In contrast, Chapter 2 takes on the problem of constructing two-qubit gate pulse sequences in a purely analytical fashion.

The main results of Chapter 2 are given in Secs. 2.3 - 2.5. Starting in Sec. 2.3, we construct a family of entangling two-qubit gate sequences [91]. These sequences consist of 39 exchange pulses, and they are therefore significantly longer than the shortest known entangling two-qubit gate sequence consisting of 18 pulses; this sequence has been found by Fong and Wandzura using a numerical search [101]. However, in Sec. 2.4 we show that an approach very similar to that followed in Sec. 2.3 can lead to the construction of another set of entangling two-qubit gate sequences
which are, at 25 pulses, only marginally longer than the Fong-Wandzura sequence. Both sequences constructed in Secs. 2.3 and 2.4 can be used to carry out controlled-phase gates.

The key idea of the constructions in Secs. 2.3 and 2.4 was to divide the large Hilbert space of the six spins that encode two three-spin qubits into smaller subspaces. These subspaces are at most two-dimensional, and can therefore be mapped onto a spin-1/2 pseudospin. We were then able to view the unitary operations due to exchange pulses as three-dimensional pseudospin rotations, allowing us to use geometric intuition to find the families of pulse sequences.

In the final and, in my view, most noteworthy part of Chapter 2 (Sec. 2.5), we provide an analytical and intuitive derivation of the shortest known two-qubit gate pulse sequence [92]. As noted above, this sequence has been found using a numerical search by Fong and Wandzura [101]. Prior to our work there was no knowledge as to how, if at all, this sequence may be understood intuitively.

To obtain the Fong-Wandzura sequence, we first evaluated a simple pulse sequence that acts on three spins and consists of a small number of elementary swap pulses. The crucial step in our derivation was then to adeptly elevate this simple sequence to a more complicated pulse sequence that acts on five spins. This elevation enabled us to directly infer the unitary operation carried out by the five-spin sequence from the operation carried out by the three-spin sequence. It was then not very difficult to show that this elevated five-spin sequence is nothing but the Fong-Wandzura sequence. This derivation is sufficiently simple that it can be carried out entirely with pen, paper, and knowledge of a few basic facts about quantum spin.

In Chapter 3 we turned to topological quantum computation where qubits are encoded using non-Abelian Fibonacci anyons. Here, quantum gates are carried out by moving anyons around one another, a process which, as explained in the introductory chapter, can be viewed as braiding the anyon worldlines in 2+1 dimensional spacetime. Part of the difficulty of the problem of finding entangling two-qubit braids stems from the nontrivial requirement that two-qubit braids need to maintain the qubit encoding. In fact, all known methods for producing two-qubit braids yield braid patterns which, when carried out, result in some error, in the sense they only maintain the qubit encoding in the limit of infinite braid length. While the problem of finding two-qubit braids has so far only been solved using methods that rely on numerical search techniques, we present the first methods for generating two-qubit braids in a systematic manner.
Our method is based on an iteration procedure for three-particle braids. This procedure, introduced by Reichardt [102], systematically generates sequences of braid patterns with operations whose matrix representations in a particular natural basis become diagonal in the limit of infinitely many iterations. Here, we show how these braids can be used in two different two-qubit braid constructions.

This Dissertation has introduced new tools into the theoretical toolkit for spin-based and anyon-based quantum computation. We expect that these new tools will have broader application in the coming years. In the next two sections we offer some speculation as to what these future applications might be.

4.2 Spin-Based Quantum Computation

When we discussed in Sec. 1.3.1 how the isotropic Heisenberg exchange interaction can be turned on and off between spins captured in semiconductor quantum dots, we said that the real spin-spin Hamiltonian will have anisotropic contributions whose terms depend strongly on the quantum dot device used in a given experiment. Furthermore, as we pointed out in Sec. 1.3.2, ideal pulse durations $t_0$ will always only be approximated by some $t_0 \pm \delta t$. Both of these effects will cause errors in the computation resulting, in the case of two-qubit gates, in both leakage-error and gate error. (A quantum gate causes leakage errors if its carrying out produces non-zero overlap of three-particle qubit states with non-computational states, defined in Secs. 2.2 for spin qubits and 3.2 for anyon qubits. Gate errors are defined by discrepancies in the unitary operations of the ideal gate and the gate carried out, after subtracting leakage errors.) This can, of course, be evaluated by subjecting the Hamiltonian and pulse durations to deviations from the ideal case when evaluating the unitary operations carried out by these errors. Leakage- and gate errors can be treated separately because there distinct procedures of correcting them. While gate errors are amended by quantum error correction schemes (see Secs. 1.1.2 and 1.2.4), leaked qubit states can be mapped back into the computational subspace using leakage correction pulse sequences. The first such sequence has been published in Ref. [101].

One reason for why the sequences discussed here have some inbuilt robustness against errors is that all of the two-qubit gate sequences of Sec. 2.3 and 2.5 are built of a sequence of smaller operations that has the form of a similarity transformation, $SU^{-1}$, where $U$ and $S$ are unitary
operations that are the result of pulse sequences. Note that removing the central operation $U$ will yield the sequence $SS^{-1}$ which results in the identity operation, and this holds if, for example, the duration of every single exchange pulse is subject to a correction of a constant, but arbitrary, $\delta t$. Some of this protection should be retained for the sequence $SUS^{-1}$. There is also reason to believe that this argument is valid for certain anisotropic corrections to the exchange Hamiltonian.

In Sec. 2.5 we have presented a class of two-qubit gate pulse sequences for which the FW sequence is optimal. Improving this limited optimality result is an interesting and important, yet complex problem. The elements of the class of two-qubit gate sequences, shown explicitly in Fig. 2.22(a), are a swap pulse (a pulse of duration $t = 1$) and a so-called $R$ sequence (introduced in Sec. 2.5.1) that acts on four spins. When applying this $R$ sequence to a three-spin qubit and a single spin there is no leakage error of the involved qubit. Therefore, a modest generalization of this class of sequences would be one for which the three appearances of $R$ are substituted by three different operations $R_1$, $R_2$, and $R_3$, none of which need to have the non-leakage property of the original $R$ operation. Similarly, the two swap pulses can be generalized to pulses of arbitrary duration. The next step would be to allow for longer sequences of these operations $R_i$ and exchange pulses, as shown in the example in Fig. 4.1(a). The interesting question to answer is whether or not the Fong Wandzura sequence is the optimal member for these generalized classes. Further, note that the two-qubit gate pulse sequences considered in Sec. 2.5 act on five of the six spins that encode two three-spin qubits. A less trivial generalization would be to consider sequences that act on all six of these spins.

Figure 4.1: (a) Generalization of the class of two-qubit pulse sequences derived in Sec. 2.5 [shown in Fig. 2.22(a)] for which we have shown in that the Fong-Wandzura sequence is the optimal member.
When comparing different sequences with each other it is important to have a clear definition of optimality. The number of required exchange pulses for a certain unitary operation depends on the spin-geometry which determines the pairs of spins that are nearest neighbors and so can undergo exchange pulses. In general, the more nearest neighbors are present the less pulses need to be carried out. For example, consider the equality of pulse sequences shown in Fig. 4.1(b). The sequence on the left-hand side effectively carries out an exchange pulse of duration $t$ between the lowermost and topmost spins for a linear array of spins. On the right-hand side, this sequence can be represented by a single “nearest-neighbor” pulse (of duration $t$) in a triangular geometry in which exchange pulses between arbitrary pairs of spins are possible. One way to define the length of a pulse sequence is then to count all pulses necessary for a fixed geometry (e.g., a linear geometry).

The analytic pulse sequence constructions given in this thesis provide an intuitive understanding of the Hilbert space of a small number of spins and the unitary operations acting this Hilbert space. As discussed in Sec. 1.3.1, there are multiple schemes for carrying out spin-based quantum computation. We believe that the insights gained by the procedures described in this thesis can be carried over to other quantum computation schemes in which pulse sequences can be useful for carrying out quantum gates or other operations, e.g., for quantum error correction procedures. For example, qubits that are encoded into more than one spin-$1/2$ particle, the problem of leakage will always have to be dealt with and for most such computation schemes there is need for certain pulse sequences. For example, for the scheme due to Levy [49] in which two-spin qubits are used, a leakage reduction sequence has been numerically determined [130]. The operation carried out by this sequence is similar to the leakage reduction sequence of Ref. [101] mentioned above. The sequence of Ref. [130] consists of exchange pulses interspersed with time intervals in which a global magnetic field is turned on. Sequences similar to this may be constructed using the intuitive understanding of the few-spin Hilbert space provided by our work.

### 4.3 Topological Quantum Computation

Above we raised the question of robustness raised above for the exchange pulse sequences established in this thesis. This question is not relevant here because, as explained in Sec. 1.3.2 and there illustrated in Fig. 1.12, the unitary operations do not depend on the details of the braid but rather only on its topology. There are thus no device-dependent corrections to the unitary
operations for anyon exchanges. Errors due to fluctuations in the environment may, of course, still occur but, since only non-local fluctuations harm the computation, errors can be strongly suppressed by keeping anyons far away from one another.

As has been pointed out in Ref. [100], a leakage-free entangling two-qubit braid would be a desirable tool for any topological quantum computation scheme based on anyons for which braiding is universal. However, a finite leakage-free two-qubit braid has not been discovered and it may very well not exist. When comparing methods for finding two-qubit anyon braids, the main point to consider is then how does the error scale as a function of the length of the braid. The braids that best approximate a desired quantum gate can simply be found via brute force search over all braids up to some finite length. For some braid length $L$, the best braids found by a brute force search result in a unitary operation $U$ approximate a desired unitary operation $U_0$ with a distance $\epsilon = |U - U_0|$ which behaves asymptotically for large length as $L \sim \log(\frac{1}{\epsilon})$. However, since the number of braids grows exponentially with the length of the braid such brute force quickly become infeasible for large braid lengths. For this reason there have been developed quite a few different procedures for process of finding two-qubit braids.

The braids described in this thesis are asymptotically optimal, that is, the braid length and leakage error follow the relationship $L \sim \log \frac{1}{\epsilon}$ and, as mentioned in Chapter 3, the method of Ref. [123] is the only other known method for constructing braids with the same optimal relationship between leakage and braid length. Now, it would be interesting to find out how exactly the leakage error versus braid length of these methods compare, that is, for $L = k \log(\frac{1}{\epsilon})$ compare the prefactor $k$ in front of the logarithm. This could be done by using both methods to construct a number of braids that approximate a particular unitary operation for different accuracies $\epsilon$, and thereby determining the corresponding prefactors.

The braids constructed here are all based on an iteration procedure of Ref. [102] which we described in Sec. 3.3. The fact that the leakage of the two-qubit braids grows optimally in the limit of small errors is rooted in the fact that this iteration generates yields braids whose unitary operations with matrix representations that converge to diagonal matrices with optimal convergence $L \sim \log(\frac{1}{\epsilon})$. It is therefore conceivable that this iteration procedure may be used in other constructions for two-qubit braids. The reason for why this would be worth considering is that the method
given in this thesis have the shortcoming that they can only be used to a small number of different number of two-qubit gates.

Finally, we would like to point out that by far the most important theoretical research to be carried out in this area is to find materials that host non-Abelian anyons for which universal quantum computation can be realized only by braiding. As an example, Mong et al. have worked out that a heterostructure of certain superconductors and Abelian Hall systems may yield Fibonacci anyons [95]. From an experimental perspective this approach seems hard to realize because quantum Hall states require relatively large magnetic fields while superconductivity breaks down for magnetic fields that are larger than the critical field. In any event, it would be very desirable to pursue research in this direction and identify new platforms towards topological quantum computation.


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BIOGRAPHICAL SKETCH

Daniel Zeuch

Education

Ph.D. Physics (expected) 9/2013 - 8/2016
Florida State University and National High Magnetic Field Laboratory Tallahassee, FL
Advisor: Nick Bonesteel

M.S. Physics 8/2011 - 8/2013
Florida State University Tallahassee, FL

University of Konstanz, Department of Physics Konstanz, Germany
Equivalent to B.S. and M.S. Physics
Diplomarbeit (Diploma Thesis): Quantum Computation with Restricted Spin Interactions
Advisor: Guido Burkard

Publications

Efficient Two-Qubit Sequences Beyond CNOT
In Preparation
Daniel Zeuch and Nick Bonesteel

Systematically Generated Two-Qubit Anyon Braids
Physical Review A 93, 052328 (2016) [arXiv:1511.00719]
Caitlin Carnahan, Daniel Zeuch and Nick Bonesteel
Simple Derivation of the Fong-Wandzura Pulse Sequence
Daniel Zeuch and Nick Bonesteel

Analytic Pulse Sequence Construction for Exchange-Only Quantum Computation
Daniel Zeuch, Robert Cipri, and Nick Bonesteel

Presentations

Systematically Generated Two-Qubit Braids for Fibonacci Anyons
APS March Meeting
Contributed Talk

Understanding the Fong-Wandzura Pulse Sequence
APS March Meeting
Contributed Talk

Two-Qubit Anyon Braids Without Brute-Force Search
QDev/NBIA 2014 Summer School
Poster Presentation

Constructing Two-Qubit Gates for Exchange-Only Quantum Computing
APS March Meeting
Contributed Talk
Pulse Sequences for Exchange-Based Quantum Computation

DPG Frühjahrstagung (Spring Meeting of the German Physical Society) Dresden, Germany
Contributed Talk

Professional Development

31st Jerusalem Winter School in Theoretical Physics Jerusalem, Israel
Frontiers of Quantum Information Science 1/2014
Attendee

Online Course at coursera.org UC Berkeley
Quantum Mechanics and Quantum Computation 10/2012
Course accomplished (with distinction)

School and Conference on Spin-Based Quantum Information Processing Konstanz, Germany 10/2010
Attendee and Assistant

Awards

Dirac Fellowship 4/2016
Department of Physics, Florida State University Tallahassee, Florida, USA
An award to recognize an outstanding piece of theoretical work