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Adiabatic Shortcut to Geometric Quantum Computation in Noiseless Subsystems

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Abstract

Quantum computers can theoretically perform certain tasks which classical computers at realistic times could not. Operating a quantum computer requires precise control over the system, for instance achieved by adiabatic evolution, and isolation from the environment to retain coherence. This report combines these two, somewhat contradicting, error preventing techniques. To reduce the run-time a transitionless quantum driving algorithm, or, adiabatic shortcut, is employed. The notion of Noiseless Subsystems (NS), a generalization of decoherence free subspaces, are used for robustness against environmental decoupling, by creating logical qubits which act as a noiseless code. Furthermore, the adiabatic shortcut for the NS code is applied to a refocusing scheme (spin-echo) in order to remove the dynamical phase, sensitive to error propagation, so that only the Berry phase is effectively picked up. The corresponding Hamiltonian is explicitly derived for the only two cases of two-dimensional NS: $N = 3, 4$ qubits with total spin of $j = 1/2, 0$, respectively. This constitutes geometric quantum computation (GQC) enacting a universal single-qubit gate, which is also explicitly derived.

Sammanfattning

Kvantdatorer kan teoretiskt utföra vissa uppgifter som klassiska datorer vid realistiska tider inte kan. Att köra en kvantdator kräver exakt kontroll över systemet, till exempel genom adiabatisk utveckling, och isolering från omgivningen för att behålla koherens. Denna rapport kombinerar dessa två, något motsägelsefulla, tekniker för felhantering. För att minska körtiden används en övergångsfri kvantkörningsalgoritm, också kallad adiabatisk genväg. Konceptet brusfria delsystem, en generalisering av dekoherensfria underrum, används för robusthet mot sammanflätning med omgivningen genom att skapa logiska kvantbitar som fungerar som en brusfri kod. Vidare tillämpas den adiabatiska genvägen för den brusfria koden på ett spinn-eko för att eliminera den dynamiska fasen, som är känslig för felpropagering, så att endast Berrys fas, som är okänslig för felpropagering, effektivt plockas upp. Motsvarande Hamiltonian härleds uttryckligen för de enda två fallen av tvådimensionella brusfria delsystem: 3 eller 4 kvantbitar med respektive totalspinn $j = 1/2$ och 0. Detta möjliggör beräkning med en geometrisk kvantdator baserad på en universell enkvantbitsgrind, som också härleds explicit.

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1 Introduction

Quantum computing (QC) holds the potential of performing certain tasks in substantially shorter time compared to what classical computers would [1]. The most famous example of this is Shor's algorithm [2] which prime-factorizes numbers in polynomial time, the difficulty of which the most prominent encryption scheme RSA is built. The dangers of rendering classical encryption schemes obsolete are handled through the field of quantum cryptography, where fundamentally safe ways of communicating information are devised [3]. This in turn suggests application such as a quantum internet. In more theoretical realms the computers would be quantum systems, and as such would naturally model quantum systems better than any classical computer, for instance enabling improved studies of material properties.

QC is performed by manipulating the wave function of the system so that when measured a desired result or solution is obtained. The manipulations are performed via so-called quantum gates which are unitary operators [4] on the qubits making up the system. Important to QC is universality, where a set of quantum gates can perform any operation. For instance the single-qubit Hadamard and phase gates, and one conditional two-qubit gate are sufficient for this. This report will only discuss single-qubit dynamics, and therefore only single-qubit universality.

The sensitive nature of the quantum regime makes the system prone to error, where tiny disturbances can render the computer useless. This report discusses methods for error prevention, although methods for error correction are also possible. There are two main challenges at present: (i) preserving coherence of the system, thus retaining the encoded information, and (ii) precise control of the system so that the desired operations can be performed, in turn solving the correct problem. This report will investigate a combination of the following solutions: (i) encoding in noiseless subsystems (NSs) [5], a generalization of decoherence-free subspaces, where an abundance of qubits form a protection against environmental influences, i.e., noise; and (ii) adiabatic shortcut [6], where the system evolves adiabatically exactly in arbitrary time, as opposed to the adiabatic approximation [7], which improves asymptotically as time of evolution tends to infinity.

An NS code with the adiabatic shortcut for spin- $\frac{1}{2}$ particles under the influence of a magnetic field is derived for both three and four physical qubits so

that a logical qubit is described. The two resulting codes are then discussed for feasible implementation, and possible further examinations are suggested. To further increase robustness a refocusing scheme called spin-echo [8] is employed to remove the dynamical phase developed and thus enabling unitaries using only Berry's phase [9]. Since Berry's phase is less sensitive to noise errors than its dynamical counterpart, the spin-echo scheme may further improve the robustness of the proposed gates.

2 Background

2.1 Qubit

Qubits are the quantum version of the classical bit. In its most general form a qubit, being a quantum system, is described as

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle, \quad (1)$$

where $\langle n|m\rangle = \delta_{nm}$ and $\alpha, \beta \in \mathbb{C}$ are the probability amplitudes fulfilling $|\alpha|^2 + |\beta|^2 = 1$, which describe with what probability a measurement would give $|0\rangle$ or $|1\rangle$. The non-descriptive aspect, apart from orthonormality, of the $\{|0\rangle, |1\rangle\}$ basis, provide the means of describing any two-level system. It could be the spin up or down of an electron $\{|\uparrow\rangle, |\downarrow\rangle\}$, the horizontal and vertical polarization of light $\{|H\rangle, |V\rangle\}$, or even a ground and excited state of energy levels $\{|g\rangle, |e\rangle\}$ in an atom or ion. In turn this fact provides multiple avenues of realising a quantum computer. Important to note is that when measured the result is either $|0\rangle$ or $|1\rangle$ and values "0" or "1", thus returning a classical value. Therefore any operations made on a qubit must be able to preserve its "quantumness".

2.2 Quantum gates

The foundation of computer operation in information processing is the enactment of logic gates on the information bits constituting the system. In QC these gates are realized through unitary operators U , i.e., $UU^\dagger = U^\dagger U = I$, with I as the identity.

Among the advantages of QC is the ability to take superpositions of qubits, of which the Hadamard gate H is the unitary most commonly employed. It

is defined as

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad (2)$$

in the computational basis, although any unitary which places the qubit in a superposition is valid. The effect on a qubit differs if it is in the $|0\rangle$ or $|1\rangle$ state as follows:

$$\begin{aligned} H|0\rangle &= \frac{|0\rangle + |1\rangle}{\sqrt{2}}, \\ H|1\rangle &= \frac{|0\rangle - |1\rangle}{\sqrt{2}}. \end{aligned} \quad (3)$$

There are also other single-qubit gates such as the Pauli-gates coinciding with the Pauli operators $\sigma_x, \sigma_y, \sigma_z$ and the phase shift gate ϕ defined as

$$\phi = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}. \quad (4)$$

The Hadamard and ϕ -gate are sufficient for all single-qubit operations in order to transform a system of n qubits into an arbitrary product state. Hence, clever combination of H and ϕ constitutes single-qubit universality.

To achieve total universality, a conditional two-qubit gate possible of entanglement is required. This report, however, will focus only on single-qubit dynamics.

2.3 Noiseless subsystem

The Hilbert \mathcal{H} space spanned by N qubits as spin-1/2 particles can be decomposed according to [10] as

$$\mathcal{H} \cong \bigoplus_j \mathbb{C}^{n_j} \otimes \mathbb{C}^{d_j}, \quad (5)$$

where j denotes the total spin, $d_j = 2J + 1$ the dimension of the subspace, and

$$n_j = \frac{N!(2j+1)}{(N/2+1+j)!(N/2-j)!} \quad (6)$$

the multiplicity of said subspace. For example in the case of $N = 2$ qubits a singlet and triplet is obtained, which is expressed in terms of the decomposition

$$\mathcal{H} = \mathbb{C}^1 \otimes \mathbb{C}^1 \oplus \mathbb{C}^1 \otimes \mathbb{C}^3. \quad (7)$$

The theory of NS is the attempt to create systems robust against global decoherence induced by the interaction with the environment. The error operators \mathcal{A} corresponding to this form of decoherence can be decomposed, similarly to the Hilbert space decomposition, as

$$\mathcal{A} \cong \bigoplus_j I_{n_j} \otimes \mathcal{M}_{d_j}. \quad (8)$$

Hence the error only affects the \mathbb{C}^{d_j} tensor-factor, meaning the subspace elements can be transformed but the multiplicity of the subspace is preserved.

In view of this, encoding information in the multiplicity would be robust against global environmental effects, i.e., noise. This can be done by creating an NS code based on operators acting as $S = S_{ns} \otimes I_{nf}$, i.e., only acting non-trivially on the multiplicity which is noiseless. This motivates the notation $|i\rangle |j, m_j\rangle_N$ for the NS-code, where $|i\rangle$ being the noiseless factor indexes the multiplicity of each subspace, $|j, m_j\rangle$ being the noisefull (nf) factor denotes a specific element of the subspace coinciding with the typical notation for a total spin state, and N the number of qubits.

The combination of NS with GQC has been demonstrated for both the adiabatic, and non-adiabatic case in [10, 11], respectively.

2.4 Adiabatic cyclic evolution

A state's parameters are more difficult to control over time than those of the Hamiltonian dictating its evolution. To have the Hamiltonian evolving the state in a controlled manner doing it slowly over a long time is of importance. This means entering the adiabatic regime. The adiabatic theorem [7] states that an eigenstate of the Hamiltonian, if evolved slowly enough, will stay in that eigenstate over the full evolution, up to a phase. For an arbitrary Hamiltonian, with instantaneous eigenstates such that

$$H_0(t) |\psi_n(t)\rangle = E_n(t) |\psi_n(t)\rangle, \quad (9)$$

the adiabatic approximation gives the states driven by $H_0(t)$ as

$$|\tilde{\psi}_n(t)\rangle = e^{i(\delta_n + \gamma_n)} |\psi_n(t)\rangle, \quad (10)$$

with the dynamical phase

$$\delta_n = -\frac{1}{\hbar} \int_0^t \langle \psi_n(t') | H_0(t') | \psi_n(t') \rangle dt', \quad (11)$$

and in the case of cyclic evolution, that is, $|\psi_n(0) = |\psi_n(T)\rangle\rangle$ for some T the geometric Berry phase [9]

$$\gamma_n = i \oint_C \langle \psi_n(\vec{R}) | \nabla_{\vec{R}} | \psi_n(\vec{R}) \rangle \cdot d\vec{R}. \quad (12)$$

Here $\vec{R}(t)$ is the parameter-vector describing the time-dependence of $|\psi_n(t)\rangle$ and traces out the path C on the Bloch sphere.

2.5 Spin-echo

In order to get a purely geometric gate, the dynamical phase must be eliminated. This would provide robustness against dynamical errors. A refocusing scheme called spin-echo [8] is employed. The method is as follows: an adiabatic evolution is traced, from which a dynamical and a Berry phase are obtained. This is done twice where the second one is done so backwards. Surrounding these evolutions are two π -transformations which flip the states (orthogonally). This is illustrated in Fig.(1). In the end both eigenstates will have picked up the same dynamical phase contribution, making it a global phase. Since that kind of phase is non-physical it can be neglected without affecting the state. The Berry phase obtained will be different for the respective eigenstates, meaning a non-trivial gate can be induced.

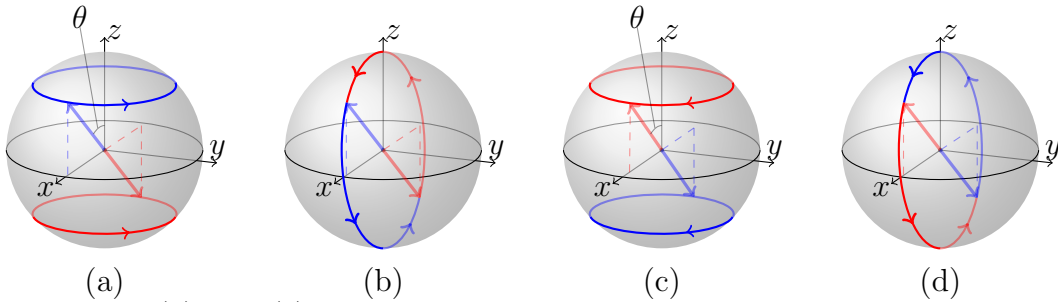


Figure 1: (a) and (c) are the two adiabatic cycles traced in opposite directions. (b) and (d) are the π -transformations, half-circle rotations around the y-axis.

2.6 Adiabatic shortcut

The great experimental challenge of adiabatic evolution is the necessarily long run-time. In order to overcome this a correctional term can be added to the Hamiltonian [6]. If $H_0(t)$ describes the adiabatic evolution as in (10), then $H(t) = H_0(t) + H_1(t)$ with

$$H_1(t) = i\hbar \sum_{m \neq n} \frac{|\psi_m\rangle\langle\psi_m| \partial_t H_0(t) |\psi_n\rangle\langle\psi_n|}{E_n - E_m} \quad (13)$$

is a transitionless Hamiltonian, meaning it evolves the eigenstates exactly for all time due to the transition amplitudes being zero. Because of this the evolution can be induced at an arbitrary speed, without the risk of losing control of the prepared state.

3 Theory and results

3.1 Noiseless code

By choosing to work with the decomposed subspaces $\mathbb{C}^{n_j} \otimes \mathbb{C}^{d_j}$ where the multiplicity $n_j = 2$, an NS-code simulating a logical qubit is can be produced. By using Eq.(6) it can be shown that the only two such cases are when using $N = 3$ and $N = 4$ qubits, and when the total spin is $j = 1/2$ and $j = 0$, respectively. Thus the two subsystems $\mathbb{C}^2 \otimes \mathbb{C}^2$ and $\mathbb{C}^2 \otimes \mathbb{C}^1$ for 3 and 4 physical qubits are obtained, respectively.

Via the Clebsch-Gordan procedure, detailed in Appendix A, with $|0\rangle := |1/2, 1/2\rangle$ and $|1\rangle := |1/2, -1/2\rangle$, the following is obtained:

$$\begin{cases} |0\rangle |1/2, 1/2\rangle_3 = \frac{1}{\sqrt{2}}(|010\rangle - |100\rangle), \\ |0\rangle |1/2, -1/2\rangle_3 = \frac{1}{\sqrt{2}}(|011\rangle - |101\rangle), \\ |1\rangle |1/2, 1/2\rangle_3 = \frac{1}{\sqrt{6}}(2|001\rangle - |010\rangle - |100\rangle), \\ |1\rangle |1/2, -1/2\rangle_3 = \frac{1}{\sqrt{6}}(|011\rangle + |101\rangle - 2|110\rangle), \end{cases} \quad (14)$$

and

$$\begin{aligned}
|0\rangle|0,0\rangle_4 &= \frac{1}{2}(|0101\rangle - |1001\rangle - |0110\rangle + |1010\rangle), \\
|1\rangle|0,0\rangle_4 &= \frac{1}{2\sqrt{3}}(2|0011\rangle - |0101\rangle - |1001\rangle - |0110\rangle - |1010\rangle + 2|1100\rangle).
\end{aligned} \tag{15}$$

The Hamiltonian used is described by the logical Pauli matrices, which are as follows:

$$\begin{aligned}
X \otimes I_{nf} &= (|1\rangle\langle 0| + |0\rangle\langle 1|) \otimes I_{nf}, \\
Y \otimes I_{nf} &= (i|1\rangle\langle 0| - i|0\rangle\langle 1|) \otimes I_{nf}, \\
Z \otimes I_{nf} &= (|0\rangle\langle 0| - |1\rangle\langle 1|) \otimes I_{nf}.
\end{aligned}$$

For a more physical expression the operators are written in terms of the permutation operators $P_{ij} = (I + \vec{\sigma}_i \cdot \vec{\sigma}_j)/2$, where $\vec{\sigma}_i = (\sigma_x, \sigma_y, \sigma_z)_i$ is the Pauli vector corresponding to the physical qubit i . This is possible because the spin and permutation operators commute, that is $[S_z, P_{ij}] = 0$, so they share eigenbasis. This substitution, described in detail in Appendix B, yield:

$$N = 3 : \begin{cases} X \otimes I_{nf} = \frac{1}{\sqrt{3}}(P_{23} - P_{13}), \\ Y \otimes I_{nf} = \frac{i}{\sqrt{3}}(P_{23}P_{13} - P_{13}P_{23}), \\ Z \otimes I_{nf} = \frac{1}{3}(P_{13} + P_{23} - 2P_{12}), \end{cases} \tag{16}$$

and

$$N = 4 : \begin{cases} X \otimes I_{nf} = \frac{1}{2\sqrt{3}}(P_{13}P_{24} - P_{14}P_{23} + P_{14} + P_{23} - P_{13} - P_{24}), \\ Y \otimes I_{nf} = \frac{i}{4\sqrt{3}}(P_{34}P_{14} + P_{24}P_{12} + P_{13}P_{12} + P_{34}P_{23} \\ \quad - P_{14}P_{34} - P_{12}P_{24} - P_{12}P_{13} - P_{23}P_{34}), \\ Z \otimes I_{nf} = \frac{1}{6}(P_{13} + P_{14} + P_{23} + P_{24} - P_{13}P_{24} - P_{14}P_{23}) \\ \quad + \frac{1}{3}(P_{12}P_{34} - P_{12} - P_{34}). \end{cases} \tag{17}$$

As a last step the operators are written in terms of the physical Pauli vectors according to the definition of the permutation operator, yielding:

$$N = 3 : \begin{cases} X \otimes I_{nf} = \frac{1}{2\sqrt{3}}(\vec{\sigma}_2 \cdot \vec{\sigma}_3 - \vec{\sigma}_1 \cdot \vec{\sigma}_3), \\ Y \otimes I_{nf} = \frac{1}{4\sqrt{3}}\vec{\sigma}_1 \cdot (\vec{\sigma}_2 \times \vec{\sigma}_3), \\ Z \otimes I_{nf} = \frac{1}{6}(\vec{\sigma}_1 \cdot \vec{\sigma}_3 + \vec{\sigma}_2 \cdot \vec{\sigma}_3 - 2\vec{\sigma}_1 \cdot \vec{\sigma}_2), \end{cases} \quad (18)$$

and

$$N = 4 : \begin{cases} X \otimes I_{nf} = \frac{1}{8\sqrt{3}}(\vec{\sigma}_1 \cdot \vec{\sigma}_4 + \vec{\sigma}_2 \cdot \vec{\sigma}_3 - \vec{\sigma}_1 \cdot \vec{\sigma}_3 - \vec{\sigma}_2 \cdot \vec{\sigma}_4 + (\vec{\sigma}_1 \times \vec{\sigma}_2) \cdot (\vec{\sigma}_3 \times \vec{\sigma}_4)), \\ Y \otimes I_{nf} = \frac{1}{8\sqrt{3}}(\vec{\sigma}_1 \cdot (\vec{\sigma}_3 \times \vec{\sigma}_4) + \vec{\sigma}_1 \cdot (\vec{\sigma}_2 \times \vec{\sigma}_3) - \vec{\sigma}_1 \cdot (\vec{\sigma}_2 \times \vec{\sigma}_4) - \vec{\sigma}_2 \cdot (\vec{\sigma}_3 \times \vec{\sigma}_4)), \\ Z \otimes I_{nf} = \frac{1}{24}(\vec{\sigma}_1 \cdot \vec{\sigma}_3 + \vec{\sigma}_1 \cdot \vec{\sigma}_4 + \vec{\sigma}_2 \cdot \vec{\sigma}_3 + \vec{\sigma}_2 \cdot \vec{\sigma}_4 + (\vec{\sigma}_1 \times \vec{\sigma}_2) \cdot (\vec{\sigma}_3 \times \vec{\sigma}_4)) \\ \quad - \frac{1}{12}(\vec{\sigma}_1 \cdot \vec{\sigma}_2 + \vec{\sigma}_3 \cdot \vec{\sigma}_4 + (\vec{\sigma}_1 \times \vec{\sigma}_4) \cdot (\vec{\sigma}_3 \times \vec{\sigma}_2)). \end{cases} \quad (19)$$

Present in Eq.(18) and Eq.(19) are Heisenberg terms $-J_{ij}(\vec{\sigma}_i \cdot \vec{\sigma}_j)$, which describe the magnetic nature of the exchange interaction between two spins. Depending on the sign of J_{ij} it is either ferromagnetic (positive) or anti-ferromagnetic (negative), which is directly related to whether the two spins are aligned or anti-aligned. This is a well-studied model regularly employed in materials science for simulations, where the spins are distributed on a lattice.

More exotic are the three-spin interactions $\vec{\sigma}_i \cdot (\vec{\sigma}_j \times \vec{\sigma}_k)$. These are anti-symmetric exchange interaction, connected to the notion of chirality [12], a sort of "handedness", where the permutation of the spins occurs in a cycle such as $|123\rangle \rightarrow |312\rangle$ or $|123\rangle \rightarrow |231\rangle$. This sort of interaction has been found to occur in single-molecule magnets, for instance [13] used an equilateral triangular setup of Cu^{2+} ions and used a chiral base similar to Eq.(18). In [14] they managed to synthesise such chiral interactions for clusters of up to 5 spins.

Even more complex are the four-spin terms $(\vec{\sigma}_i \times \vec{\sigma}_j) \cdot (\vec{\sigma}_k \times \vec{\sigma}_l)$. These terms have come up in four-spin cyclic exchange phenomena, which have been

studied in spin-ladder models as a coupling between vector chiralities [15, 16]. The terms have for instance been observed contributing in a significant manner to the magnetic properties of manganites in [17].

3.2 Adiabatic shortcut to spin-echo

To obtain a Hamiltonian with an adiabatic shortcut the following starting Hamiltonian is defined:

$$H_0(t) = \gamma \vec{B}_0(t) \cdot \vec{S}, \quad (20)$$

where γ is the gyromagnetic ratio and

$$\vec{S} = \frac{\hbar}{2} \vec{\Sigma} = \frac{\hbar}{2} (X, Y, Z), \quad (21)$$

the spin vector. Moreover, define

$$\vec{b}_0(t) := \frac{\vec{B}_0(t)}{|\vec{B}_0(t)|} = \frac{\vec{B}_0(t)}{B_0(t)}, \quad (22)$$

as the direction of the magnetic field. As shown in [6] the correction Hamiltonian Eq.(13) takes the form

$$H_1(t) = (\vec{b}_0(t) \times \partial_t \vec{b}_0(t)) \cdot \vec{S}. \quad (23)$$

The total Hamiltonian inducing a transitionless evolution is therefore

$$H(t) = (\gamma \vec{B}_0(t) + \vec{b}_0(t) \times \partial_t \vec{b}_0(t)) \cdot \vec{S} =: \gamma \vec{B}(t) \cdot \vec{S}. \quad (24)$$

The direction of the magnetic can generally be expressed as:

$$\vec{b}_0(t) = (\sin \theta \cos \omega t, \sin \theta \sin \omega t, \cos \theta), \quad (25)$$

which in turn yields the total magnetic field

$$\begin{aligned} \vec{B}(t) = & \left(B_0 - \frac{1}{\gamma} \omega \cos \theta \right) \sin \theta (\hat{e}_x \cos \omega t + \hat{e}_y \sin \omega t) \\ & + \left(B_0 \cos \theta + \frac{1}{\gamma} \omega \sin^2 \theta \right) \hat{e}_z, \end{aligned} \quad (26)$$

where from now on the field strength $B_0(t) = B_0$ is taken to be constant. This leads to the transitionless Hamiltonian

$$\begin{aligned} H(t) = & \frac{\hbar}{2} (\gamma B_0 - \omega \cos \theta) \sin \theta \cos(\omega t) X \\ & + \frac{\hbar}{2} (\gamma B_0 - \omega \cos \theta) \sin \theta \sin(\omega t) Y \\ & + \frac{\hbar}{2} (\gamma B_0 \cos \theta + \omega \sin^2 \theta) Z. \end{aligned} \quad (27)$$

By defining

$$\begin{aligned} \omega_0 &:= \gamma B_0 \cos \theta + \omega \sin^2 \theta, \\ \omega_1 &:= (\gamma B_0 - \omega \cos \theta) \sin \theta, \end{aligned} \quad (28)$$

the Hamiltonian (27) simplifies to

$$\begin{aligned} H(t) &= \frac{\hbar}{2} \omega_1 \cos(\omega t) X + \frac{\hbar}{2} \omega_1 \sin(\omega t) Y + \frac{\hbar}{2} \omega_0 Z \\ &= \frac{\hbar}{2} [\omega_1 (\cos(\omega t) X + \sin(\omega t) Y) + \omega_0 Z]. \end{aligned} \quad (29)$$

The refocusing sequence, as described earlier is

$$C \rightarrow \pi \rightarrow \tilde{C} \rightarrow \pi, \quad (30)$$

where C is the path traced by the eigenstates $|\psi_n(t)\rangle$ of the Hamiltonian $H_0(t)$ driven by $H(t)$, and $\tilde{C}(\omega) = C(-\omega)$ is the same path traced backwards. The π transformation is enacted after each cycle and described by the Hamiltonian

$$H(t) = \gamma \vec{B}_\pi(t) \cdot \hat{S}, \quad (31)$$

with

$$\gamma \vec{B}_\pi(t) = (0, \omega_\pi, 0), \quad (32)$$

and so

$$H(t) = \frac{\hbar}{2} \omega_\pi Y. \quad (33)$$

The sequence can now be described by a Hamiltonian divided up as

$$H(t) = \begin{cases} H^{(1)}(t) & , \quad 0 \leq t \leq \frac{2\pi}{\omega}, \\ H^{(2)}(t) & , \quad t_1 \leq t \leq t_1 + \frac{\pi}{\omega_\pi}, \\ H^{(3)}(t) & , \quad t_2 \leq t \leq t_2 + \frac{2\pi}{\omega}, \\ H^{(4)}(t) & , \quad t_3 \leq t \leq t_3 + \frac{\pi}{\omega_\pi} \equiv \tau, \end{cases} \quad (34)$$

where $t_1 > \frac{2\pi}{\omega}$, $t_2 > t_1 + \frac{\pi}{\omega_\pi}$, and $t_3 > t_2 + \frac{2\pi}{\omega}$. Worth noting again is that the states driven are not the eigenstates of $H(t)$ but of $H_0(t)$. The shortcut obtained enables the evolution to exactly track the instantaneous eigenstates of $H_0(t)$, even though the evolution is performed in non-adiabatic time. A consequence of this is that the Berry phase is unaffected by the shortcut, apart from being picked up faster.

The magnetic fields corresponding to the cyclic paths will have different opening angles, meaning that a change in angle to the rotational axis will have to be made in the lab, however the field-strength the same for both evolutions. By defining the difference of the magnetic fields to be their relative vector, $\vec{B}^{(13)} := \vec{B}^{(1)} - \vec{B}^{(3)} = \frac{2}{\gamma}\omega \sin \theta (-\cos \theta \cos \omega t, \cos \theta \sin \omega t, \sin \theta)$ is obtained. Note that the relative vector scales with ω , meaning the speed at which the evolution is traced dictates the difference in magnetic fields. This is a direct consequence of the adiabatic shortcut since the ω factor arose from the correction term, it can also be seen since the adiabatic approximation is letting $\omega \ll 1$ and the relative vector would be close to zero, thus neglected. The respective magnitudes do not differ because $|\vec{B}^{(1)}| = |\vec{B}^{(3)}| = B_0 \sqrt{1 + \left(\frac{\omega}{\gamma B_0} \sin \theta\right)^2}$ is unaffected by a sign change of ω . The discussed aspects are illustrated below in Fig.(2).

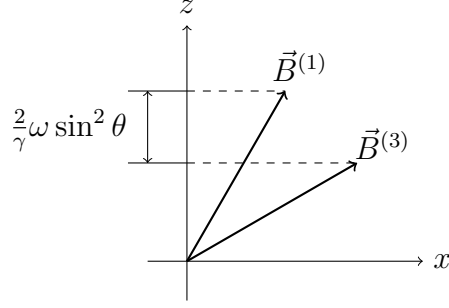


Figure 2: The difference in magnetic field for the first and second cycle, in the xz -plane.

In the following subsections the Hamiltonian from Eq.(34) is expressed explicitly for the 3 and 4 physical qubits respectively constituting the NS code.

3.2.1 3 physical qubits, $j = 1/2$

Substituting for the Pauli operators X, Y, Z in the previously derived code Eq.(18) yields

$$\begin{aligned}
 H(t) = & \frac{\hbar}{2}\omega_1 \left(\cos(\omega t) \frac{1}{2\sqrt{3}} (\vec{\sigma}_2 \cdot \vec{\sigma}_3 - \vec{\sigma}_1 \cdot \vec{\sigma}_3) + \sin(\omega t) \frac{1}{4\sqrt{3}} \vec{\sigma}_1 \cdot (\vec{\sigma}_2 \times \vec{\sigma}_3) \right) \\
 & + \frac{\hbar}{2}\omega_0 \frac{1}{6} (\vec{\sigma}_1 \cdot \vec{\sigma}_3 + \vec{\sigma}_2 \cdot \vec{\sigma}_3 - 2\vec{\sigma}_1 \cdot \vec{\sigma}_2)
 \end{aligned} \tag{35}$$

and gathering terms result in

$$\begin{aligned}
 H^{(1)}(t) = & -\frac{\hbar}{6}\omega_0 \vec{\sigma}_1 \cdot \vec{\sigma}_2 \\
 & + \frac{\hbar}{12} (\omega_0 - \sqrt{3}\omega_1 \cos(\omega t)) \vec{\sigma}_1 \cdot \vec{\sigma}_3 \\
 & + \frac{\hbar}{12} (\omega_0 + \sqrt{3}\omega_1 \cos(\omega t)) \vec{\sigma}_2 \cdot \vec{\sigma}_3 \\
 & + \frac{\hbar}{8\sqrt{3}}\omega_1 \sin(\omega t) \vec{\sigma}_1 \cdot (\vec{\sigma}_2 \times \vec{\sigma}_3).
 \end{aligned} \tag{36}$$

For $H^{(3)}(t)$, where $\omega \rightarrow -\omega$, define $\tilde{\omega}_{0,1}(\omega) := \omega_{0,1}(-\omega)$, yielding

$$\begin{aligned}
H^{(3)}(t) = & -\frac{\hbar}{6}\tilde{\omega}_0\vec{\sigma}_1 \cdot \vec{\sigma}_2 \\
& + \frac{\hbar}{12}(\tilde{\omega}_0 - \sqrt{3}\tilde{\omega}_1\cos(\omega t))\vec{\sigma}_1 \cdot \vec{\sigma}_3 \\
& + \frac{\hbar}{12}(\tilde{\omega}_0 + \sqrt{3}\tilde{\omega}_1\cos(\omega t))\vec{\sigma}_2 \cdot \vec{\sigma}_3 \\
& - \frac{\hbar}{8\sqrt{3}}\tilde{\omega}_1\sin(\omega t)\vec{\sigma}_1 \cdot (\vec{\sigma}_2 \times \vec{\sigma}_3).
\end{aligned} \tag{37}$$

The π -transformation is simply

$$H^{(2)}(t) = H^{(4)}(t) = \frac{\hbar\omega_\pi}{8\sqrt{3}}\vec{\sigma}_1 \cdot (\vec{\sigma}_2 \times \vec{\sigma}_3). \tag{38}$$

The interactions of the spins are illustrated below in Fig.(3).

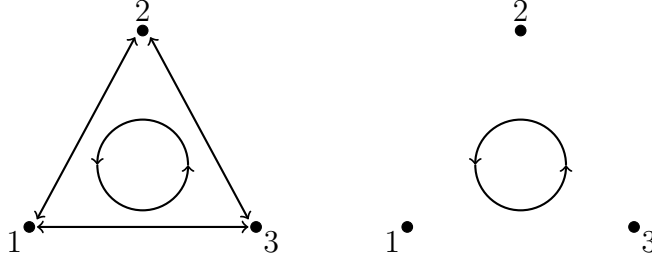


Figure 3: The dots represent the physical qubits. The left diagram represents the interactions of the path C induced by $H^{(1)}(t)$ and $H^{(3)}(t)$. The right diagram represents the π -transformation of $H^{(2)}(t)$ and $H^{(4)}(t)$. The straight arrows correspond to the Heisenberg interaction. The circle shows the chiral interaction, where the direction is determined by the sign.

3.2.2 4 physical qubits, $j = 0$

The same procedure but for the $j = 0$ Pauli operators yields

$$\begin{aligned}
H = & \frac{\hbar}{16\sqrt{3}}\omega_1 \cos(\omega t) \\
& \times (\vec{\sigma}_1 \cdot \vec{\sigma}_4 + \vec{\sigma}_2 \cdot \vec{\sigma}_3 - \vec{\sigma}_1 \cdot \vec{\sigma}_3 - \vec{\sigma}_2 \cdot \vec{\sigma}_4 + (\vec{\sigma}_1 \times \vec{\sigma}_2) \cdot (\vec{\sigma}_3 \times \vec{\sigma}_4)) \\
& + \frac{\hbar}{16\sqrt{3}}\omega_1 \sin(\omega t) \\
& \times (\vec{\sigma}_1 \cdot (\vec{\sigma}_3 \times \vec{\sigma}_4) + \vec{\sigma}_1 \cdot (\vec{\sigma}_2 \times \vec{\sigma}_3) - \vec{\sigma}_1 \cdot (\vec{\sigma}_2 \times \vec{\sigma}_4) - \vec{\sigma}_2 \cdot (\vec{\sigma}_3 \times \vec{\sigma}_4)) \\
& + \frac{\hbar}{48}\omega_0 \\
& \times (\vec{\sigma}_1 \cdot \vec{\sigma}_3 + \vec{\sigma}_1 \cdot \vec{\sigma}_4 + \vec{\sigma}_2 \cdot \vec{\sigma}_3 + \vec{\sigma}_2 \cdot \vec{\sigma}_4 + (\vec{\sigma}_1 \times \vec{\sigma}_2) \cdot (\vec{\sigma}_3 \times \vec{\sigma}_4) \\
& - 2(\vec{\sigma}_1 \cdot \vec{\sigma}_2 + \vec{\sigma}_3 \cdot \vec{\sigma}_4 + (\vec{\sigma}_1 \times \vec{\sigma}_4) \cdot (\vec{\sigma}_3 \times \vec{\sigma}_2))).
\end{aligned} \tag{39}$$

Gathering interaction terms,

$$\begin{aligned}
H = & -\frac{\hbar}{24}\omega_0 \vec{\sigma}_1 \cdot \vec{\sigma}_2 \\
& + \frac{\hbar}{48}(\omega_0 - \sqrt{3}\omega_1 \cos(\omega t)) \vec{\sigma}_1 \cdot \vec{\sigma}_3 \\
& + \frac{\hbar}{48}(\omega_0 + \sqrt{3}\omega_1 \cos(\omega t)) \vec{\sigma}_1 \cdot \vec{\sigma}_4 \\
& + \frac{\hbar}{48}(\omega_0 + \sqrt{3}\omega_1 \cos(\omega t)) \vec{\sigma}_2 \cdot \vec{\sigma}_3 \\
& + \frac{\hbar}{48}(\omega_0 - \sqrt{3}\omega_1 \cos(\omega t)) \vec{\sigma}_2 \cdot \vec{\sigma}_4 \\
& - \frac{\hbar}{24}\omega_0 \vec{\sigma}_3 \cdot \vec{\sigma}_4 \\
& + \frac{\hbar}{16\sqrt{3}}\omega_1 \sin(\omega t)(\vec{\sigma}_1 \cdot (\vec{\sigma}_3 \times \vec{\sigma}_4) + \vec{\sigma}_1 \cdot (\vec{\sigma}_2 \times \vec{\sigma}_3)) \\
& - \frac{\hbar}{16\sqrt{3}}\omega_1 \sin(\omega t)(\vec{\sigma}_1 \cdot (\vec{\sigma}_2 \times \vec{\sigma}_4) + \vec{\sigma}_2 \cdot (\vec{\sigma}_3 \times \vec{\sigma}_4)) \\
& + \frac{\hbar}{48}(\omega_0 + \sqrt{3}\omega_1 \cos(\omega t))(\vec{\sigma}_1 \times \vec{\sigma}_2) \cdot (\vec{\sigma}_3 \times \vec{\sigma}_4) \\
& - \frac{\hbar}{24}\omega_0(\vec{\sigma}_1 \times \vec{\sigma}_4) \cdot (\vec{\sigma}_3 \times \vec{\sigma}_2),
\end{aligned} \tag{40}$$

and finally gather coefficients to obtain

$$\begin{aligned}
H^{(1)}(t) = & \frac{\hbar}{48} \left(\omega_0 + \sqrt{3}\omega_1 \cos(\omega t) \right) (\vec{\sigma}_1 \cdot \vec{\sigma}_4 + \vec{\sigma}_2 \cdot \vec{\sigma}_3 + (\vec{\sigma}_1 \times \vec{\sigma}_2) \cdot (\vec{\sigma}_3 \times \vec{\sigma}_4)) \\
& + \frac{\hbar}{48} \left(\omega_0 - \sqrt{3}\omega_1 \cos(\omega t) \right) (\vec{\sigma}_1 \cdot \vec{\sigma}_3 + \vec{\sigma}_2 \cdot \vec{\sigma}_4) \\
& + \frac{\hbar}{16\sqrt{3}} \omega_1 \sin(\omega t) (\vec{\sigma}_1 \cdot (\vec{\sigma}_3 \times \vec{\sigma}_4) + \vec{\sigma}_1 \cdot (\vec{\sigma}_2 \times \vec{\sigma}_3)) \\
& - \frac{\hbar}{16\sqrt{3}} \omega_1 \sin(\omega t) (\vec{\sigma}_1 \cdot (\vec{\sigma}_2 \times \vec{\sigma}_4) + \vec{\sigma}_2 \cdot (\vec{\sigma}_3 \times \vec{\sigma}_4)) \\
& - \frac{\hbar}{24} \omega_0 (\vec{\sigma}_1 \cdot \vec{\sigma}_2 + \vec{\sigma}_3 \cdot \vec{\sigma}_4 + (\vec{\sigma}_1 \times \vec{\sigma}_4) \cdot (\vec{\sigma}_3 \times \vec{\sigma}_2)).
\end{aligned} \tag{41}$$

The counter-rotating path is therefore

$$\begin{aligned}
H^{(3)}(t) = & \frac{\hbar}{48} \left(\tilde{\omega}_0 + \sqrt{3}\tilde{\omega}_1 \cos(\omega t) \right) (\vec{\sigma}_1 \cdot \vec{\sigma}_4 + \vec{\sigma}_2 \cdot \vec{\sigma}_3 + (\vec{\sigma}_1 \times \vec{\sigma}_2) \cdot (\vec{\sigma}_3 \times \vec{\sigma}_4)) \\
& + \frac{\hbar}{48} \left(\tilde{\omega}_0 - \sqrt{3}\tilde{\omega}_1 \cos(\omega t) \right) (\vec{\sigma}_1 \cdot \vec{\sigma}_3 + \vec{\sigma}_2 \cdot \vec{\sigma}_4) \\
& - \frac{\hbar}{16\sqrt{3}} \tilde{\omega}_1 \sin(\omega t) (\vec{\sigma}_1 \cdot (\vec{\sigma}_3 \times \vec{\sigma}_4) + \vec{\sigma}_1 \cdot (\vec{\sigma}_2 \times \vec{\sigma}_3)) \\
& + \frac{\hbar}{16\sqrt{3}} \tilde{\omega}_1 \sin(\omega t) (\vec{\sigma}_1 \cdot (\vec{\sigma}_2 \times \vec{\sigma}_4) + \vec{\sigma}_2 \cdot (\vec{\sigma}_3 \times \vec{\sigma}_4)) \\
& - \frac{\hbar}{24} \tilde{\omega}_0 (\vec{\sigma}_1 \cdot \vec{\sigma}_2 + \vec{\sigma}_3 \cdot \vec{\sigma}_4 + (\vec{\sigma}_1 \times \vec{\sigma}_4) \cdot (\vec{\sigma}_3 \times \vec{\sigma}_2)).
\end{aligned} \tag{42}$$

The π -transformations are

$$\begin{aligned}
H^{(2)}(t) = H^{(4)}(t) = & \frac{\hbar\omega_\pi}{16\sqrt{3}} (\vec{\sigma}_1 \cdot (\vec{\sigma}_3 \times \vec{\sigma}_4) + \vec{\sigma}_1 \cdot (\vec{\sigma}_2 \times \vec{\sigma}_3) \\
& - \vec{\sigma}_1 \cdot (\vec{\sigma}_2 \times \vec{\sigma}_4) - \vec{\sigma}_2 \cdot (\vec{\sigma}_3 \times \vec{\sigma}_4)).
\end{aligned} \tag{43}$$

The interactions of the spins are illustrated below in Fig.(4).

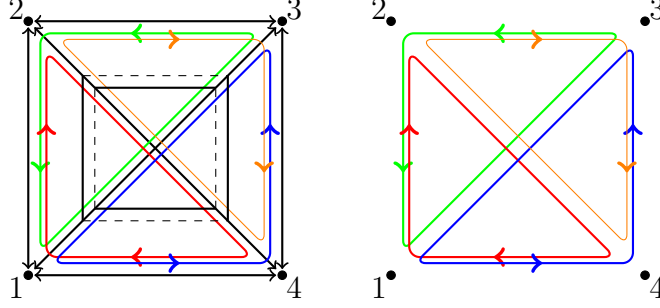


Figure 4: The dots represent the physical qubits. The left diagram represents the interactions of the path C induced by $H^{(1)}(t)$ and $H^{(3)}(t)$. The right diagram represents the π -transformation of $H^{(2)}(t)$ and $H^{(4)}(t)$. The straight arrows correspond to the Heisenberg interaction. The colored triangles shows the chiral 3-spin interactions, where the direction is determined by the sign. The squares show the 4-spin interactions of coupled vector chiralities.

3.3 Single-qubit gates

Exploiting the Berry phase enacting single-qubit gates is possible. First the original Hamiltonian

$$H_0(t) = \frac{\hbar\gamma B_0}{2} \begin{pmatrix} \cos \theta & \sin \theta e^{-i\omega t} \\ \sin \theta e^{i\omega t} & -\cos \theta \end{pmatrix} \quad (44)$$

diagonalizes to

$$\begin{aligned} |\psi_0(t)\rangle &= \cos \frac{\theta}{2} |0\rangle + \sin \frac{\theta}{2} e^{i\omega t} |1\rangle, & E_0 &= \frac{\hbar\gamma B_0}{2}, \\ |\psi_1(t)\rangle &= -\sin \frac{\theta}{2} |0\rangle + \cos \frac{\theta}{2} e^{i\omega t} |1\rangle, & E_1 &= -\frac{\hbar\gamma B_0}{2}. \end{aligned} \quad (45)$$

Notice the time-dependence of the eigenstates is solely in the $e^{i\omega t}$ factor. As mentioned previously this motivates a time-dependence parameter-vector, in this case $\vec{R} = \omega t =: \varphi$ with the cyclic path $\varphi \in [0, 2\pi]$. Hence, the Berry phases γ_x ($x = 0, 1$) obtained are:

$$\begin{aligned} \gamma_0 &= \oint_C i \langle \psi_0 | \nabla_R | \psi_0 \rangle \cdot d\vec{R} \\ &= i \int_0^{2\pi} \left(\cos \frac{\theta}{2} \langle 0 | + \sin \frac{\theta}{2} e^{-i\varphi} \langle 1 | \right) i \sin \frac{\theta}{2} e^{i\varphi} | 1 \rangle d\varphi \\ &= -\pi(1 - \cos \theta), \end{aligned} \quad (46)$$

and

$$\begin{aligned}
\gamma_1 &= \oint_C i \langle \psi_1 | \nabla_R | \psi_1 \rangle \cdot d\vec{R} \\
&= i \int_0^{2\pi} \left(-\sin \frac{\theta}{2} \langle 0 | + \cos \frac{\theta}{2} e^{-i\varphi} \langle 1 | \right) i \cos \frac{\theta}{2} e^{i\varphi} | 1 \rangle d\varphi \\
&= -\pi(1 + \cos \theta).
\end{aligned} \tag{47}$$

Two observations can be made. First, these are the phases acquired by the corresponding eigenstates of $H_0(t)$ evolving with the Hamiltonian $H^{(1)}(t)$ as previously described. The corresponding phase for the orthogonal evolution $H^{(3)}(t)$ would be calculated simply by changing the sign on the upper limit of the integration, thus resulting only in an overall sign change. If the first evolution is denoted by C_x and the second, backwards, evolution \tilde{C}_x , then the phases acquired would be γ_x and $\tilde{\gamma}_x$, respectively, hence $\tilde{\gamma}_x = -\gamma_x$.

Second, the phases can be related to the solid angle $\Omega = 2\pi(1 - \cos \theta)$ of the traced out paths of $|\psi_0\rangle$ and $|\psi_1\rangle$. It can be directly observed that $\gamma_0 = -\Omega/2$. The second phase can be worked out as $\gamma_1 = -2\pi + \Omega/2$. Since these phases are actually expressed in exponentials as $e^{i\gamma_x}$, there is redundancy in any additional factor of 2π , that is they describe the same physics since $e^{i\gamma_1} = e^{i(-2\pi + \Omega/2)} = e^{-i2\pi} e^{i\Omega/2} = e^{i\Omega/2}$. In view of this the Berry phases can be expressed as

$$\gamma_x = \left(x - \frac{1}{2}\right)\Omega. \tag{48}$$

Applying these two observations to the refocusing scheme yield

$$\begin{aligned}
|\psi_x\rangle &\xrightarrow{C_x} e^{i(\delta_x + \gamma_x)} |\psi_x\rangle \xrightarrow{\pi} e^{i(\delta_x + \gamma_x)} |\psi_{x\oplus 1}\rangle \\
&\xrightarrow{\tilde{C}_x} e^{i(\delta_x + \delta_{x\oplus 1} + \gamma_x - \gamma_{x\oplus 1})} |\psi_{x\oplus 1}\rangle \\
&\xrightarrow{\pi} e^{i(\delta_x + \delta_{x\oplus 1} + \gamma_x - \gamma_{x\oplus 1})} |\psi_x\rangle,
\end{aligned} \tag{49}$$

where \oplus is addition mod 2. The dynamical contribution is identical for both starting eigenstates because the shortcut does not contribute to the phase, which can be seen by calculation of the correction Hamiltonian inte-

grands:

$$\begin{aligned}
\langle \psi_0(t) | H_1(t) | \psi_0(t) \rangle &= \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} e^{i\omega t} \end{pmatrix}^\dagger \frac{\hbar\omega \sin \theta}{2} \begin{pmatrix} \sin \theta & -\cos \theta e^{-i\omega t} \\ -\cos \theta e^{i\omega t} & -\sin \theta \end{pmatrix} \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} e^{i\omega t} \end{pmatrix} \\
&= \frac{\hbar\omega \sin \theta}{2} \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} e^{i\omega t} \end{pmatrix}^\dagger \begin{pmatrix} -\sin \frac{\theta}{2} \\ \cos \frac{\theta}{2} e^{i\omega t} \end{pmatrix} \\
&= \frac{\hbar\omega \sin \theta}{2} \left(-\cos \frac{\theta}{2} \sin \frac{\theta}{2} + \sin \frac{\theta}{2} \cos \frac{\theta}{2} \right) = 0, \\
\langle \psi_1(t) | H_1(t) | \psi_1(t) \rangle &= \begin{pmatrix} -\sin \frac{\theta}{2} \\ \cos \frac{\theta}{2} e^{i\omega t} \end{pmatrix}^\dagger \frac{\hbar\omega \sin \theta}{2} \begin{pmatrix} \sin \theta & -\cos \theta e^{-i\omega t} \\ -\cos \theta e^{i\omega t} & -\sin \theta \end{pmatrix} \begin{pmatrix} -\sin \frac{\theta}{2} \\ \cos \frac{\theta}{2} e^{i\omega t} \end{pmatrix} \\
&= \frac{\hbar\omega \sin \theta}{2} \begin{pmatrix} -\sin \frac{\theta}{2} \\ \cos \frac{\theta}{2} e^{i\omega t} \end{pmatrix}^\dagger \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} e^{i\omega t} \end{pmatrix} \\
&= \frac{\hbar\omega \sin \theta}{2} \left(-\cos \frac{\theta}{2} \sin \frac{\theta}{2} + \sin \frac{\theta}{2} \cos \frac{\theta}{2} \right) = 0.
\end{aligned} \tag{50}$$

This is the same as $\langle \psi_x(t) | H_1(t) | \psi_x(t) \rangle = \frac{\hbar}{2} \omega \sin \theta \langle \psi_x(t) | \psi_{x \oplus 1}(t) \rangle = 0$, meaning $\langle \psi_x(t) | H(t) | \psi_x(t) \rangle = \langle \psi_x(t) | H_0(t) | \psi_x(t) \rangle$, and so the dynamical phases are unaffected. Moreover, the total contribution is a global phase and can be neglected. In the eigenbasis $\{|\psi_0\rangle, |\psi_1\rangle\}$ the transformation (49) corresponds to the phase gate $\Phi_\Omega : |\psi_x\rangle \rightarrow U(\Omega) |\psi_x\rangle = e^{i(x-\frac{1}{2})2\Omega} |\psi_x\rangle$, i.e.,

$$U(\Omega) = e^{-i\Omega} |\psi_0\rangle\langle\psi_0| + e^{i\Omega} |\psi_1\rangle\langle\psi_1|. \tag{51}$$

Rewriting this in terms of the computational basis $\{|0\rangle, |1\rangle\}$ via the expressions for the eigenstates and, which is of great importance, setting $t = 0$ to obtain the instantaneous eigenstates which are acted upon in the scheme, yield the unitary

$$U(\theta, \Omega) = \begin{pmatrix} \cos^2 \frac{\theta}{2} e^{-i\Omega} + \sin^2 \frac{\theta}{2} e^{i\Omega} & -i \sin \theta \sin \Omega \\ -i \sin \theta \sin \Omega & \sin^2 \frac{\theta}{2} e^{-i\Omega} + \cos^2 \frac{\theta}{2} e^{i\Omega} \end{pmatrix}, \tag{52}$$

or $U(\theta, \Omega) = e^{-i\Omega \vec{n} \cdot \vec{\Sigma}}$, where $\vec{n} = (\sin \theta, 0, \cos \theta)$. For $U(\theta, \Omega)$ to be universal θ and Ω must be able to vary independently, but as previously defined $\Omega(\theta) = 2\pi(1 - \cos \theta)$, and so another ϑ is required. This can be obtained by rotating the magnetic field around some symmetry axis, in this case the y -axis [18]

(or by changing basis as was done in [19]) such that: $\vec{B}' = R_y(\vartheta - \theta)\vec{B}$, in turn producing the rotated direction $\vec{n}' = R_y(\vartheta - \theta)\vec{n}$, i.e.,

$$\vec{n}' = \begin{pmatrix} \cos(\vartheta - \theta) & 0 & \sin(\vartheta - \theta) \\ 0 & 1 & 0 \\ -\sin(\vartheta - \theta) & 0 & \cos(\vartheta - \theta) \end{pmatrix} \begin{pmatrix} \sin \theta \\ 0 \\ \cos \theta \end{pmatrix} = \begin{pmatrix} \sin \vartheta \\ 0 \\ \cos \vartheta \end{pmatrix}. \quad (53)$$

The result is the universal unitary

$$U(\vartheta, \Omega) = \begin{pmatrix} \cos^2 \frac{\vartheta}{2} e^{-i\Omega} + \sin^2 \frac{\vartheta}{2} e^{i\Omega} & -i \sin \vartheta \sin \Omega \\ -i \sin \vartheta \sin \Omega & \sin^2 \frac{\vartheta}{2} e^{-i\Omega} + \cos^2 \frac{\vartheta}{2} e^{i\Omega} \end{pmatrix}, \quad (54)$$

where, by definition, ϑ and Ω can now be varied independently. Moreover, due to the spherical symmetry the Berry phases remains the same. This is because the same path is traced, only in a rotated frame, and as such the solid angles remains the same.

For two unitaries U_1, U_2 to contribute to universality it is necessary that $[U_1, U_2] \neq 0$, which can be shown to equate to

$$\sin \Omega_1 \sin \Omega_2 \sin(\vartheta_1 - \vartheta_2) \neq 0. \quad (55)$$

Simply choosing $\vartheta_1 - \vartheta_2 \neq 0 \pm n\pi$, where $n \in \mathbb{Z}$, takes care of the issue. By letting $\vartheta_1 = 0$ the unitary

$$U_1(0, \Omega_1) = \begin{pmatrix} e^{-i\Omega_1} & 0 \\ 0 & e^{i\Omega_1} \end{pmatrix}, \quad (56)$$

is obtained which is equivalent to the ϕ -gate up to a global phase $e^{i\Omega_1}$. Now for the second gate, let $\vartheta_2 = \pi/2$, then

$$U_2\left(\frac{\pi}{2}, \Omega_2\right) = \begin{pmatrix} \cos \Omega_2 & -i \sin \Omega_2 \\ -i \sin \Omega_2 & \cos \Omega_2 \end{pmatrix}. \quad (57)$$

Furthermore, either set $\Omega_2 = \pi/2$ to obtain the equivalent to spin-flip

$$U_2\left(\frac{\pi}{2}, \frac{\pi}{2}\right) = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}. \quad (58)$$

up to the phase $e^{3i\pi/2}$, or set $\Omega_2 = \pi/4$ to obtain

$$U_2\left(\frac{\pi}{2}, \frac{\pi}{4}\right) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix}. \quad (59)$$

which is a so-called "equal weighted superposition gate", the same type of gate as in Eq.(2), the Hadamard gate.

4 Outlook

The scheme should be extended to include two-qubit interactions in order to achieve universality. This could be done for instance via an Ising model as previously done in [8] for a single physical qubit undergoing adiabatic evolution.

Experimental testing of the derived systems is naturally of interest.

The magnetic field used in this report was assumed to have constant strength. Consequences of letting it vary in time could be explored, perhaps leading to simpler expressions.

The NS code with adiabatic shortcut can be applied to other schemes than spin-echo. It can also be used on non-adiabatic schemes.

5 Conclusions

Quantum computers hold the potential to change the information processing landscape. To realize these machines certain obstacles, such as error prevention, need addressing. The notion of noiseless subsystems was used to construct the two possible codes capable of simulating a single logical qubit resilient against global entanglement to an environment. An adiabatic shortcut leading to transitionless driving of eigenstates was implemented alongside the noiseless code to perform geometric quantum computation via a refocusing sequence, or, spin echo, in turn eliminating the dynamical phase so that only the Berry phase remained. Furthermore, two universal sets of single-qubit unitaries were explicitly derived. Thus several errors have been prevented, where the system is robust against environmental effects, random local parameter fluctuations, and perhaps most importantly, the run-time required for this security has been eliminated due to the adiabatic shortcut. Observed in the NS code were the three- and four-spin interactions connected to scalar and vector chirality, interactions observed in single molecular magnets, 2D quantum solids and more. Several avenues of continued research related to the derived code and implementation have been suggested, such as, extending the scheme to include two-qubit gates and experimentally test the proposed gates.

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A Qubit addition

Denote $|0\rangle = |1/2, 1/2\rangle$ and $|1\rangle = |1/2, -1/2\rangle$ and $|i\rangle \otimes |j\rangle = |ij\rangle$. The lowering operator S_- will be used to obtain the superposition of states that describes the total state vector. It acts on a state as follows $S_- |s, m\rangle = \hbar C_- |s, m-1\rangle$ with $C_- = \sqrt{(s+m)(s-m+1)}$ being the Clebsch-Gordan coefficients. The total state is generally expressed as

$$|s_1, s_2; s, m\rangle_N = \sum_{m_1, m_2} \langle s_1, m_1; s_2, m_2 | s_1, s_2; s, m \rangle |s_1, m_1; s_2, m_2\rangle$$

where the inner products are the C_- 's and N denotes the number of qubits. The lowering operator for the total state is the sum of the lowering operator for the separate states as follows $S_- = S_{1-} \otimes \hat{1} + \hat{1} \otimes S_{2-}$, this implies that the \hbar factor will appear on both sides of the equation and can therefore be omitted from the calculations. To begin with, calculate the operation on the qubits $|0\rangle, |1\rangle$. The $|1\rangle$ will just equal zero since it's the lowest state. For $|0\rangle$ $C_- = 1$ so $S_- |0\rangle = \hbar |1\rangle$, and since \hbar is omitted lowering a single spin-1/2 is generated by the Pauli lowering operator $\sigma_- = |1\rangle \langle 0|$.

The method to obtain all the total states for n qubits will be to start with the highest possible state from $|s_1 - s_2| \leq s \leq |s_1 + s_2|$ and define it as $|s = s_1 + s_2, m\rangle = |0\rangle_1 \otimes \dots \otimes |0\rangle_N$

2 qubits

Add two $s = 1/2$, which gives $s = 0, 1$. Starting with $s = 1$

$$|1, 1\rangle_2 = |00\rangle$$

acting with lowering operator yield

$$\begin{aligned} S_- |1, 1\rangle_2 &= (S_{1-} \otimes \hat{1} + \hat{1} \otimes S_{2-}) |00\rangle \\ \Rightarrow \sqrt{2} |1, 0\rangle_2 &= |10\rangle + |01\rangle \\ \Leftrightarrow |1, 0\rangle_2 &= \frac{1}{\sqrt{2}}(|10\rangle + |01\rangle) \end{aligned}$$

and lowering once again to get

$$\begin{aligned}
S_- |1, 0\rangle_2 &= (S_{1-} \otimes \hat{1} + \hat{1} \otimes S_{2-}) \frac{1}{\sqrt{2}}(|10\rangle + |01\rangle) \\
\Rightarrow \sqrt{2} |1, -1\rangle_2 &= \frac{2}{\sqrt{2}} |11\rangle \\
\Leftrightarrow |1, -1\rangle_2 &= |11\rangle
\end{aligned}$$

The lowest possible state is expected to be a single term of the lowest states of the qubits, since this process works analogously by using the raising operator starting from the lowest possible state.

The triplet has been obtained, there is also a singlet for the case $s = 0$ i.e. $|0, 0\rangle$. Compare with the state with same m , that is $|1, 0\rangle$ and try to construct an orthogonal total state. By choosing

$$|0, 0\rangle_2 = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle),$$

the singlet and triplet for 2 qubits are

$$\begin{aligned}
|0, 0\rangle_2 &= \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle) \\
\left\{ \begin{aligned} |1, 1\rangle_2 &= |00\rangle \\ |1, 0\rangle_2 &= \frac{1}{\sqrt{2}}(|10\rangle + |01\rangle) \\ |1, -1\rangle_2 &= |11\rangle \end{aligned} \right.
\end{aligned}$$

3 qubits

For $N \geq 3$ number of qubits start with the same process as for the $N = 2$ case, that is begin with the highest possible state and then use the lowering operator, followed by finding orthogonal states for lower s . But the results from lower N can be reused to get around a lot of the calculations by adding the qubit to the different subspaces, e.g. the triplet. For $N = 3$ that looks like

$$|3/2, 3/2\rangle_3 = |000\rangle = |1, 1\rangle_2 \otimes |0\rangle$$

since the lowering operator acting on $|1, 1\rangle_2$ has already been calculated it simplifies things,

$$\begin{aligned}\sqrt{3}|3/2, 1/2\rangle_3 &= \sqrt{2}|1, 0\rangle_2 \otimes |0\rangle + |1, 1\rangle_2 \otimes |1\rangle \\ \Leftrightarrow |3/2, 1/2\rangle_3 &= \frac{1}{\sqrt{3}}(\sqrt{2}|1, 0\rangle_2 \otimes |0\rangle + |1, 1\rangle_2 \otimes |1\rangle).\end{aligned}$$

The procedure continues until the lowest state,

$$\begin{aligned}2|3/2, -1/2\rangle_3 &= \frac{1}{\sqrt{3}}(2|1, -1\rangle_2 \otimes |0\rangle + \sqrt{2}|1, 0\rangle_2 \otimes |1\rangle + \sqrt{2}|1, 0\rangle_2 \otimes |1\rangle) \\ \Leftrightarrow |3/2, -1/2\rangle_3 &= \frac{1}{\sqrt{3}}(|1, -1\rangle_2 \otimes |0\rangle + \sqrt{2}|1, 0\rangle_2 \otimes |1\rangle),\end{aligned}$$

and

$$\begin{aligned}\sqrt{3}|3/2, -3/2\rangle_3 &= \frac{3}{\sqrt{3}}|1, -1\rangle_2 \otimes |1\rangle \\ \Leftrightarrow |3/2, -3/2\rangle_3 &= |1, -1\rangle_2 \otimes |1\rangle.\end{aligned}$$

Thus the quadruplet has been obtained. Now for the doublet. Examine $|3/2, 1/2\rangle$ to see what anti-symmetry can be made in order to construct the $|1/2, 1/2\rangle$ state vector, just as in the $N = 2$ case.

$$|3/2, 1/2\rangle_3 = \frac{1}{\sqrt{3}}(\sqrt{2}|1, 0\rangle_2 \otimes |0\rangle + |1, 1\rangle_2 \otimes |1\rangle)$$

choose

$$|1/2, 1/2\rangle_3 = \frac{1}{\sqrt{3}}(\sqrt{2}|1, 1\rangle_2 \otimes |1\rangle - |1, 0\rangle_2 \otimes |0\rangle),$$

and lowering to get

$$\begin{aligned}|1/2, -1/2\rangle_3 &= \frac{1}{\sqrt{3}}(2|1, 0\rangle_2 \otimes |1\rangle - \sqrt{2}|1, -1\rangle_2 \otimes |0\rangle - |1, 0\rangle_2 \otimes |1\rangle) \\ &= \frac{1}{\sqrt{3}}(|1, 0\rangle_2 \otimes |1\rangle - \sqrt{2}|1, -1\rangle_2 \otimes |0\rangle).\end{aligned}$$

Finally add a qubit to the singlet to obtain some $|1/2, 1/2\rangle_3$ state vector

$$|1/2, 1/2\rangle_3 = |0, 0\rangle_2 \otimes |0\rangle,$$

and lowering to get

$$|1/2, -1/2\rangle_3 = |0, 0\rangle_2 \otimes |1\rangle.$$

At last substitute in the $N = 2$ states to get the two doublets and the quadruplet

$$\left\{ \begin{array}{l} |0\rangle |1/2, 1/2\rangle_3 = \frac{1}{\sqrt{2}}(|010\rangle - |100\rangle), \\ |0\rangle |1/2, -1/2\rangle_3 = \frac{1}{\sqrt{2}}(|011\rangle - |101\rangle), \\ |1\rangle |1/2, 1/2\rangle_3 = \frac{1}{\sqrt{6}}(2|001\rangle - |010\rangle - |100\rangle), \\ |1\rangle |1/2, -1/2\rangle_3 = \frac{1}{\sqrt{6}}(|011\rangle + |101\rangle - 2|110\rangle), \\ |0\rangle |3/2, 3/2\rangle_3 = |000\rangle, \\ |0\rangle |3/2, 1/2\rangle_3 = \frac{1}{\sqrt{3}}(|001\rangle + |010\rangle + |100\rangle), \\ |0\rangle |3/2, -1/2\rangle_3 = \frac{1}{\sqrt{3}}(|011\rangle + |101\rangle + |110\rangle), \\ |0\rangle |3/2, -3/2\rangle_3 = |111\rangle. \end{array} \right.$$

4 qubits

As done in the $N = 3$ case we use the previous results to form the new total state vectors:

$$|2, 2\rangle_4 = |0000\rangle = |3/2, 3/2\rangle_3 \otimes |0\rangle,$$

and lowering to get

$$\begin{aligned} 2|2, 1\rangle_4 &= \sqrt{3}|3/2, 1/2\rangle_3 \otimes |0\rangle + |3/2, 3/2\rangle_3 \otimes |1\rangle \\ \Leftrightarrow |2, 1\rangle_4 &= \frac{1}{2}(\sqrt{3}|3/2, 1/2\rangle_3 \otimes |0\rangle + |3/2, 3/2\rangle_3 \otimes |1\rangle) \\ \Rightarrow \sqrt{6}|2, 0\rangle_4 &= \frac{1}{2}(2\sqrt{3}|3/2, -1/2\rangle_3 \otimes |0\rangle + \sqrt{3}|3/2, 1/2\rangle_3 \otimes |1\rangle + \sqrt{3}|3/2, 1/2\rangle_3 \otimes |1\rangle) \\ |2, 0\rangle_4 &= \frac{1}{\sqrt{2}}(|3/2, 1/2\rangle_3 \otimes |1\rangle + |3/2, -1/2\rangle_3 \otimes |0\rangle) \end{aligned}$$

$$\begin{aligned}
\Rightarrow \sqrt{6} |2, -1\rangle_4 &= \frac{1}{\sqrt{2}} (2 |3/2, -1/2\rangle_3 \otimes |1\rangle + \sqrt{3} |3/2, -3/2\rangle_3 \otimes |0\rangle + |3/2, -1/2\rangle_3 \otimes |1\rangle) \\
&\Leftrightarrow |2, -1\rangle_4 = \frac{1}{2} (\sqrt{3} |3/2, -1/2\rangle_3 \otimes |1\rangle + |3/2, -3/2\rangle_3 \otimes |0\rangle) \\
\Rightarrow 2 |2, -2\rangle_4 &= \frac{1}{2} (3 |3/2, -3/2\rangle_3 \otimes |1\rangle + |3/2, -3/2\rangle_3 \otimes |1\rangle) \\
&\Leftrightarrow |2, -2\rangle_4 = |3/2, -3/2\rangle_3 \otimes |1\rangle.
\end{aligned}$$

To get the corresponding $|1, 1\rangle_4$ compare to $|2, 1\rangle_4$, from which it can be seen that

$$|1, 1\rangle_4 = \frac{1}{2} (\sqrt{3} |3/2, 3/2\rangle_3 \otimes |1\rangle - |3/2, 1/2\rangle_3 \otimes |0\rangle)$$

and lowering to get

$$\begin{aligned}
\sqrt{2} |1, 0\rangle_4 &= \frac{1}{2} (3 |3/2, 1/2\rangle_3 \otimes |1\rangle - 2 |3/2, -1/2\rangle_3 \otimes |0\rangle - |3/2, 1/2\rangle_3 \otimes |1\rangle) \\
&\Leftrightarrow |1, 0\rangle_4 = \frac{1}{\sqrt{2}} (|3/2, 1/2\rangle_3 \otimes |1\rangle - |3/2, -1/2\rangle_3 \otimes |0\rangle) \\
\Rightarrow \sqrt{2} |1, -1\rangle_4 &= \frac{1}{\sqrt{2}} (2 |3/2, -1/2\rangle_3 \otimes |1\rangle - \sqrt{3} |3/2, -3/2\rangle_3 \otimes |0\rangle - |3/2, -1/2\rangle_3 \otimes |1\rangle) \\
&\Leftrightarrow |1, -1\rangle_4 = \frac{1}{2} (|3/2, -1/2\rangle_3 \otimes |1\rangle - \sqrt{3} |3/2, -3/2\rangle_3 \otimes |0\rangle)
\end{aligned}$$

Now to add a qubit to the doublets. With the employed procedure, the resulting states will be identical until substitution, and so it is only required to do once. Start with

$$|1, 1\rangle_4 = |1/2, 1/2\rangle_3 \otimes |0\rangle$$

and lower to get

$$\begin{aligned}
\sqrt{2} |1, 0\rangle_4 &= |1/2, -1/2\rangle_3 \otimes |0\rangle + |1/2, 1/2\rangle_3 \otimes |1\rangle \\
&\Leftrightarrow |1, 0\rangle_4 = \frac{1}{\sqrt{2}} (|1/2, -1/2\rangle_3 \otimes |0\rangle + |1/2, 1/2\rangle_3 \otimes |1\rangle) \\
\Rightarrow \sqrt{2} |1, -1\rangle_4 &\Leftrightarrow \frac{1}{\sqrt{2}} (|1/2, -1/2\rangle_3 \otimes |1\rangle + |1/2, -1/2\rangle_3 \otimes |1\rangle) \\
&|1, -1\rangle_4 = |1/2, -1/2\rangle_3 \otimes |1\rangle.
\end{aligned}$$

The corresponding $|0, 0\rangle_4$ is

$$|0,0\rangle_4 = \frac{1}{\sqrt{2}}(|1/2, 1/2\rangle_3 \otimes |1\rangle - |1/2, -1/2\rangle_3 \otimes |0\rangle).$$

All subspaces have now been expressed and the proper substitutions from the $N = 3$ results can be made to obtain the 2 singlets, 3 triplets, and 1 quintuplet:

$$\begin{aligned} |0\rangle |0,0\rangle_4 &= \frac{1}{2}(|0101\rangle - |1001\rangle - |0110\rangle + |1010\rangle), \\ |1\rangle |0,0\rangle_4 &= \frac{1}{2\sqrt{3}}(2|0011\rangle - |0101\rangle - |1001\rangle - |0110\rangle - |1010\rangle + 2|1100\rangle), \\ \left\{ \begin{aligned} |0\rangle |1,1\rangle_4 &= \frac{1}{\sqrt{6}}(2|0010\rangle - |0100\rangle - |1000\rangle), \\ |0\rangle |1,0\rangle_4 &= \frac{1}{2\sqrt{3}}(2|0011\rangle - |0101\rangle - |1001\rangle + |0110\rangle + |1010\rangle - 2|1100\rangle), \\ |0\rangle |1,-1\rangle_4 &= \frac{1}{\sqrt{6}}(|0111\rangle + |1011\rangle - 2|1101\rangle), \end{aligned} \right. \\ \left\{ \begin{aligned} |1\rangle |1,1\rangle_4 &= \frac{1}{2\sqrt{3}}(3|0001\rangle - |0010\rangle - |0100\rangle - |1000\rangle), \\ |1\rangle |1,0\rangle_4 &= \frac{1}{\sqrt{6}}(|0011\rangle + |0101\rangle + |1001\rangle - |0110\rangle - |1010\rangle - |1100\rangle), \\ |1\rangle |1,-1\rangle_4 &= \frac{1}{2\sqrt{3}}(|0111\rangle + |1011\rangle + |1101\rangle - 3|1110\rangle), \end{aligned} \right. \\ \left\{ \begin{aligned} |2\rangle |1,1\rangle_4 &= \frac{1}{\sqrt{2}}(|0100\rangle - |1000\rangle), \\ |2\rangle |1,0\rangle_4 &= \frac{1}{2}(|0101\rangle - |1001\rangle + |0110\rangle - |1010\rangle), \\ |2\rangle |1,-1\rangle_4 &= \frac{1}{\sqrt{2}}(|0111\rangle - |1011\rangle), \end{aligned} \right. \\ \left\{ \begin{aligned} |0\rangle |2,2\rangle_4 &= |0000\rangle, \\ |0\rangle |2,1\rangle_4 &= \frac{1}{2}(|0001\rangle + |0010\rangle + |0100\rangle + |1000\rangle), \\ |0\rangle |2,0\rangle_4 &= \frac{1}{\sqrt{6}}(|0011\rangle + |0101\rangle + |1001\rangle + |0110\rangle + |1010\rangle + |1100\rangle), \\ |0\rangle |2,-1\rangle_4 &= \frac{1}{2}(|0111\rangle + |1011\rangle + |1101\rangle + |1110\rangle), \\ |0\rangle |2,-2\rangle_4 &= |1111\rangle. \end{aligned} \right. \end{aligned}$$

B Permutation operators

The Permutation operators P_{ij} are of interest to express the Hamiltonians used in more physical terms than spin operators. This is possible because the permutation operator $P_{ij} = (I_{ij} + \vec{\sigma}_i \cdot \vec{\sigma}_j)/2 \otimes I = (|00\rangle\langle 00| + |11\rangle\langle 11| + |01\rangle\langle 10| + |10\rangle\langle 01|)_{ij} \otimes I$, with $\vec{\sigma}_i = (\sigma_x, \sigma_y, \sigma_z)_i$ (the identity tensor factor acts on the other indices), commutes with the spin operator S_z . This means they share a common eigenbasis, therefore the states can be expanded in terms of permutations instead of the spin states. In both cases $N = 3$ and $N = 4$ the Hamiltonian is in terms of the Pauli matrices like so:

$$\begin{aligned} X \otimes I_{nf} &= (|1\rangle\langle 0| + |0\rangle\langle 1|) \otimes I_{nf} \\ Y \otimes I_{nf} &= (i|1\rangle\langle 0| - i|0\rangle\langle 1|) \otimes I_{nf} \\ Z \otimes I_{nf} &= (|0\rangle\langle 0| - |1\rangle\langle 1|) \otimes I_{nf} \end{aligned}$$

General relation

For two permutation operators taken together which combined act on 3 qubits 3-qubit the following relations are true,

$$\begin{cases} P_{ik}P_{ij} - P_{ij}P_{ik} = \frac{1}{2i}\vec{\sigma}_i \cdot (\vec{\sigma}_j \times \vec{\sigma}_k) \\ P_{jk}P_{ij} - P_{ij}P_{jk} = \frac{i}{2}\vec{\sigma}_i \cdot (\vec{\sigma}_j \times \vec{\sigma}_k) \\ P_{jk}P_{ik} - P_{ik}P_{jk} = \frac{1}{2i}\vec{\sigma}_i \cdot (\vec{\sigma}_j \times \vec{\sigma}_k) \end{cases}$$

with $i < j < k$ and proven below. In this report $i, j, k, l \in \{1, 2, 3, 4\}$ where depending on if it is the 3 or 4 qubit system there will be a $\hat{1}_l$ tensor factor which will not affect the system, so it is omitted. The cyclic relation $\sigma_a \cdot \sigma_b = \epsilon_{abc}\sigma_c$ where $a, b, c \in x, y, z$ and ϵ_{abc} is the Levi-Civita symbol will be used. It is only required show one of these relations, proven by assuming the first relation hold to get

$$\begin{aligned} P_{ik}P_{ij} - P_{ij}P_{ik} &= P_{ki}P_{ji} - P_{ji}P_{ki} \\ i &\rightarrow k \\ k &\rightarrow j \\ j &\rightarrow i \\ \Rightarrow P_{jk}P_{ik} - P_{ik}P_{jk} &= \frac{1}{2i}\vec{\sigma}_k \cdot (\vec{\sigma}_i \times \vec{\sigma}_j) \end{aligned}$$

The circular relation of triple yield

$$P_{jk}P_{ik} - P_{ik}P_{jk} = \frac{1}{2i}\vec{\sigma}_k \cdot (\vec{\sigma}_i \times \vec{\sigma}_j) = \frac{1}{2i}\vec{\sigma}_i \cdot (\vec{\sigma}_j \times \vec{\sigma}_k),$$

and

$$\begin{aligned} P_{ik}P_{ij} - P_{ij}P_{ik} &= P_{ik}P_{ji} - P_{ji}P_{ik} \\ &\quad \begin{matrix} i \rightarrow j \\ j \rightarrow i \end{matrix} \\ \Rightarrow P_{jk}P_{ij} - P_{ij}P_{jk} &= \frac{1}{2i}\vec{\sigma}_j \cdot (\vec{\sigma}_i \times \vec{\sigma}_k) \end{aligned}$$

Permutation of any two operators in a triple product is anti-symmetry so,

$$P_{jk}P_{ij} - P_{ij}P_{jk} = \frac{1}{2i}\vec{\sigma}_j \cdot (\vec{\sigma}_i \times \vec{\sigma}_k) = \frac{i}{2}\vec{\sigma}_i \cdot (\vec{\sigma}_j \times \vec{\sigma}_k).$$

The first relation is derived below.

$$\begin{aligned} P_{ik}P_{ij} - P_{ij}P_{ik} &= \frac{1}{4}(I + \vec{\sigma}_i \cdot \vec{\sigma}_k)(I + \vec{\sigma}_i \cdot \vec{\sigma}_j) - \frac{1}{4}(I + \vec{\sigma}_i \cdot \vec{\sigma}_j)(I + \vec{\sigma}_i \cdot \vec{\sigma}_k) \\ &= \frac{1}{4}[(\vec{\sigma}_i \cdot \vec{\sigma}_k)(\vec{\sigma}_i \cdot \vec{\sigma}_j) - (\vec{\sigma}_i \cdot \vec{\sigma}_j)(\vec{\sigma}_i \cdot \vec{\sigma}_k)] \\ &= \frac{1}{4}[(\sigma_x \otimes \hat{1} \otimes \sigma_x + \sigma_y \otimes \hat{1} \otimes \sigma_y + \sigma_z \otimes \hat{1} \otimes \sigma_z) \\ &\quad \times (\sigma_x \otimes \sigma_x \otimes \hat{1} + \sigma_y \otimes \sigma_y \otimes \hat{1} + \sigma_z \otimes \sigma_z \otimes \hat{1}) \\ &\quad - (\sigma_x \otimes \sigma_x \otimes \hat{1} + \sigma_y \otimes \sigma_y \otimes \hat{1} + \sigma_z \otimes \sigma_z \otimes \hat{1}) \\ &\quad \times (\sigma_x \otimes \hat{1} \otimes \sigma_x + \sigma_y \otimes \hat{1} \otimes \sigma_y + \sigma_z \otimes \hat{1} \otimes \sigma_z)] \\ &= \frac{1}{4}[\sigma_x^2 \otimes \sigma_x \otimes \sigma_x + \sigma_x \sigma_y \otimes \sigma_y \otimes \sigma_x + \sigma_x \sigma_z \otimes \sigma_z \otimes \sigma_x \\ &\quad + \sigma_y \sigma_x \otimes \sigma_x \otimes \sigma_y + \sigma_y^2 \otimes \sigma_y \otimes \sigma_y + \sigma_y \sigma_z \otimes \sigma_z \otimes \sigma_y \\ &\quad + \sigma_z \sigma_x \otimes \sigma_x \otimes \sigma_z + \sigma_z \sigma_y \otimes \sigma_y \otimes \sigma_z + \sigma_z^2 \otimes \sigma_z \otimes \sigma_z \\ &\quad - (\sigma_x^2 \otimes \sigma_x \otimes \sigma_x + \sigma_y \sigma_x \otimes \sigma_y \otimes \sigma_x + \sigma_z \sigma_x \otimes \sigma_z \otimes \sigma_x \\ &\quad + \sigma_x \sigma_y \otimes \sigma_x \otimes \sigma_y + \sigma_y^2 \otimes \sigma_y \otimes \sigma_y + \sigma_z \sigma_y \otimes \sigma_z \otimes \sigma_y \\ &\quad + \sigma_x \sigma_z \otimes \sigma_x \otimes \sigma_z + \sigma_y \sigma_z \otimes \sigma_y \otimes \sigma_z + \sigma_z^2 \otimes \sigma_z \otimes \sigma_z)] \end{aligned}$$

$$\begin{aligned}
&= \frac{1}{4} [\hat{1} \otimes \sigma_x \otimes \sigma_x + i\sigma_z \otimes \sigma_y \otimes \sigma_x - i\sigma_y \otimes \sigma_z \otimes \sigma_x \\
&\quad - i\sigma_z \otimes \sigma_x \otimes \sigma_y + \hat{1} \otimes \sigma_y \otimes \sigma_y + i\sigma_x \otimes \sigma_z \otimes \sigma_y \\
&\quad + i\sigma_y \otimes \sigma_x \otimes \sigma_z - i\sigma_x \otimes \sigma_y \otimes \sigma_z + \hat{1} \otimes \sigma_z \otimes \sigma_z \\
&\quad - (\hat{1} \otimes \sigma_x \otimes \sigma_x - i\sigma_z \otimes \sigma_y \otimes \sigma_x + i\sigma_y \otimes \sigma_z \otimes \sigma_x \\
&\quad + i\sigma_z \otimes \sigma_x \otimes \sigma_y + \hat{1} \otimes \sigma_y \otimes \sigma_y - i\sigma_x \otimes \sigma_z \otimes \sigma_y \\
&\quad - i\sigma_y \otimes \sigma_x \otimes \sigma_z + i\sigma_x \otimes \sigma_y \otimes \sigma_z + \hat{1} \otimes \sigma_z \otimes \sigma_z)] \\
&= \frac{i}{2} (\sigma_x \otimes \sigma_z \otimes \sigma_y + \sigma_y \otimes \sigma_x \otimes \sigma_z + \sigma_z \otimes \sigma_y \otimes \sigma_x \\
&\quad - \sigma_x \otimes \sigma_y \otimes \sigma_z - \sigma_y \otimes \sigma_z \otimes \sigma_x - \sigma_z \otimes \sigma_x \otimes \sigma_y) \\
&= \frac{-i}{2} \begin{vmatrix} \sigma_x & \sigma_y & \sigma_z \\ \sigma_x & \sigma_y & \sigma_z \\ \sigma_x & \sigma_y & \sigma_z \end{vmatrix} \\
&= \frac{1}{2i} \vec{\sigma}_i \cdot (\vec{\sigma}_j \times \vec{\sigma}_k)
\end{aligned}$$

3 qubits

The permutation operators are:

$$\begin{aligned}
P_{12} &= |010\rangle\langle 100| + |000\rangle\langle 000| + |110\rangle\langle 110| + |100\rangle\langle 010| \\
&\quad + |011\rangle\langle 101| + |001\rangle\langle 001| + |111\rangle\langle 111| + |101\rangle\langle 011| \\
P_{13} &= |000\rangle\langle 000| + |111\rangle\langle 111| + |101\rangle\langle 101| + |100\rangle\langle 001| \\
&\quad + |001\rangle\langle 100| + |010\rangle\langle 010| + |110\rangle\langle 011| + |011\rangle\langle 110| \\
P_{23} &= |000\rangle\langle 000| + |111\rangle\langle 111| + |011\rangle\langle 011| + |010\rangle\langle 001| \\
&\quad + |001\rangle\langle 010| + |100\rangle\langle 100| + |110\rangle\langle 101| + |101\rangle\langle 110| \\
I &= |000\rangle\langle 000| + |001\rangle\langle 001| + |010\rangle\langle 010| + |100\rangle\langle 100| \\
&\quad + |011\rangle\langle 011| + |101\rangle\langle 101| + |110\rangle\langle 110| + |111\rangle\langle 111|
\end{aligned}$$

Hence the following:

$$\begin{aligned}
X \otimes I_{nf} &= \frac{1}{\sqrt{3}}(P_{23} - P_{13}) \\
Z \otimes I_{nf} &= \frac{1}{3}(P_{13} + P_{23} - 2P_{12}).
\end{aligned}$$

Use commutation relations to get the representation for $Y \otimes I_{nf}$ since $[Z \otimes I_{nf}, X \otimes I_{nf}] = [Z, X] \otimes I_{nf} = 2i \cdot Y \otimes I_{nf}$. We find

$$\begin{aligned}
Y \otimes I_{nf} &= \frac{1}{2i}[Z \otimes I_{nf}, X \otimes I_{nf}] \\
&= \frac{1}{2i} \left(\frac{1}{\sqrt{3}}(P_{23} - P_{13}) \frac{1}{3}(P_{13} + P_{23} - 2P_{12}) - \frac{1}{3}(P_{13} + P_{23} - 2P_{12}) \frac{1}{\sqrt{3}}(P_{23} - P_{13}) \right) \\
&= \frac{i}{6\sqrt{3}} ((P_{13} + P_{23} - 2P_{12})(P_{23} - P_{13}) - (P_{23} - P_{13})(P_{13} + P_{23} - 2P_{12})) \\
&= \frac{i}{6\sqrt{3}} (P_{23}P_{13} + P_{23}P_{23} - 2P_{23}P_{12} - P_{13}P_{13} - P_{13}P_{23} + 2P_{13}P_{12} \\
&\quad - P_{13}P_{23} + P_{13}P_{13} - P_{23}P_{23} + P_{23}P_{13} + P_{12}P_{23} - 2P_{12}P_{13})
\end{aligned}$$

Simplify by gathering terms and using $P_{ij}P_{ij} = I$, since permuting two objects twice is the same as having done nothing, i.e., identity. This yields

$$\begin{aligned}
Y \otimes I_{nf} &= \frac{i}{6\sqrt{3}} (2P_{23}P_{13} - 2P_{23}P_{12} - 2P_{13}P_{23} + 2P_{13}P_{12} \\
&\quad + 2P_{12}P_{23} - 2P_{12}P_{13}).
\end{aligned}$$

Investigate the action of the operators on a general vector:

$$\begin{aligned}
P_{23}P_{13}(1, 2, 3) &= P_{23}(3, 2, 1) = (3, 1, 2) \\
P_{23}P_{12}(1, 2, 3) &= P_{23}(2, 1, 3) = (2, 3, 1) \\
P_{12}P_{13}(1, 2, 3) &= P_{12}(3, 2, 1) = (2, 3, 1) \\
P_{12}P_{23}(1, 2, 3) &= P_{12}(1, 3, 2) = (3, 1, 2) \\
P_{13}P_{23}(1, 2, 3) &= P_{13}(1, 3, 2) = (2, 3, 1) \\
P_{13}P_{12}(1, 2, 3) &= P_{13}(2, 1, 3) = (3, 1, 2)
\end{aligned}$$

Notice that $P_{23}P_{12} = P_{12}P_{13} = P_{13}P_{23}$ and $P_{23}P_{13} = P_{12}P_{23} = P_{13}P_{12}$, therefore the final result is

$$Y \otimes I_{nf} = \frac{i}{\sqrt{3}}(P_{23}P_{13} - P_{13}P_{23}).$$

In summary, for N=3 physical qubits the Pauli operators are:

$$\begin{cases}
X \otimes I_{nf} = \frac{1}{\sqrt{3}}(P_{23} - P_{13}) \\
Y \otimes I_{nf} = \frac{i}{\sqrt{3}}(P_{23}P_{13} - P_{13}P_{23}) \\
Z \otimes I_{nf} = \frac{1}{3}(P_{13} + P_{23} - 2P_{12}).
\end{cases}$$

Furthermore, the true interest is to express these through Heisenberg interaction terms $\vec{\sigma}_i \cdot \vec{\sigma}_j$. This is done by substituting the P_{ij} with their definition, with the identity tensor factor $\hat{1}$ omitted, to obtain

$$\begin{cases}
X \otimes I_{nf} = \frac{1}{2\sqrt{3}}(\vec{\sigma}_2 \cdot \vec{\sigma}_3 - \vec{\sigma}_1 \cdot \vec{\sigma}_3) \\
Y \otimes I_{nf} = \frac{1}{4\sqrt{3}}\vec{\sigma}_1 \cdot (\vec{\sigma}_2 \times \vec{\sigma}_3) \\
Z \otimes I_{nf} = \frac{1}{6}(\vec{\sigma}_1 \cdot \vec{\sigma}_3 + \vec{\sigma}_2 \cdot \vec{\sigma}_3 - 2\vec{\sigma}_1 \cdot \vec{\sigma}_2).
\end{cases}$$

4 qubits

The permutation operators are:

$$\begin{aligned}
P_{12} &= |0000\rangle\langle 0000| + |0011\rangle\langle 0011| + |0001\rangle\langle 0001| + |0010\rangle\langle 0010| \\
&\quad + |1100\rangle\langle 1100| + |1111\rangle\langle 1111| + |1101\rangle\langle 1101| + |1110\rangle\langle 1110| \\
&\quad + |0100\rangle\langle 1000| + |0111\rangle\langle 1011| + |0101\rangle\langle 1001| + |0110\rangle\langle 1010| \\
&\quad + |1000\rangle\langle 0100| + |1011\rangle\langle 0111| + |1001\rangle\langle 0101| + |1010\rangle\langle 0110| \\
P_{13} &= |0000\rangle\langle 0000| + |0101\rangle\langle 0101| + |0001\rangle\langle 0001| + |0100\rangle\langle 0100| \\
&\quad + |1010\rangle\langle 1010| + |1111\rangle\langle 1111| + |1011\rangle\langle 1011| + |1110\rangle\langle 1110| \\
&\quad + |0010\rangle\langle 1000| + |0111\rangle\langle 1101| + |0011\rangle\langle 1001| + |0110\rangle\langle 1100| \\
&\quad + |1000\rangle\langle 0010| + |1101\rangle\langle 0111| + |1001\rangle\langle 0011| + |1100\rangle\langle 0110| \\
P_{14} &= |0000\rangle\langle 0000| + |0110\rangle\langle 0110| + |0010\rangle\langle 0010| + |0100\rangle\langle 0100| \\
&\quad + |1001\rangle\langle 1001| + |1111\rangle\langle 1111| + |1011\rangle\langle 1011| + |1101\rangle\langle 1101| \\
&\quad + |0001\rangle\langle 1000| + |0111\rangle\langle 1110| + |0011\rangle\langle 1010| + |0101\rangle\langle 1100| \\
&\quad + |1000\rangle\langle 0001| + |1110\rangle\langle 0111| + |1010\rangle\langle 0011| + |1100\rangle\langle 0101| \\
P_{23} &= |0000\rangle\langle 0000| + |1001\rangle\langle 1001| + |0001\rangle\langle 0001| + |1000\rangle\langle 1000| \\
&\quad + |0110\rangle\langle 0110| + |1111\rangle\langle 1111| + |0111\rangle\langle 0111| + |1110\rangle\langle 1110| \\
&\quad + |0010\rangle\langle 0100| + |1011\rangle\langle 1101| + |0011\rangle\langle 0101| + |1010\rangle\langle 1100| \\
&\quad + |0100\rangle\langle 0010| + |1101\rangle\langle 1011| + |0101\rangle\langle 0011| + |1100\rangle\langle 1010| \\
P_{24} &= |0000\rangle\langle 0000| + |1010\rangle\langle 1010| + |0010\rangle\langle 0010| + |1000\rangle\langle 1000| \\
&\quad + |0101\rangle\langle 0101| + |1111\rangle\langle 1111| + |0111\rangle\langle 0111| + |1101\rangle\langle 1101| \\
&\quad + |0001\rangle\langle 0100| + |1011\rangle\langle 1110| + |0011\rangle\langle 0110| + |1001\rangle\langle 1100| \\
&\quad + |0100\rangle\langle 0001| + |1110\rangle\langle 1011| + |0110\rangle\langle 0011| + |1100\rangle\langle 1001| \\
P_{34} &= |0000\rangle\langle 0000| + |1100\rangle\langle 1100| + |0100\rangle\langle 0100| + |1000\rangle\langle 1000| \\
&\quad + |0011\rangle\langle 0011| + |1111\rangle\langle 1111| + |0111\rangle\langle 0111| + |1011\rangle\langle 1011| \\
&\quad + |0001\rangle\langle 0010| + |1101\rangle\langle 1110| + |0101\rangle\langle 0110| + |1001\rangle\langle 1010| \\
&\quad + |0010\rangle\langle 0001| + |1110\rangle\langle 1101| + |0110\rangle\langle 0101| + |1010\rangle\langle 1001| \\
I &= |0000\rangle\langle 0000| + |0001\rangle\langle 0001| + |0010\rangle\langle 0010| + |0100\rangle\langle 0100| \\
&\quad + |1000\rangle\langle 1000| + |0011\rangle\langle 0011| + |0101\rangle\langle 0101| + |1001\rangle\langle 1001| \\
&\quad + |0110\rangle\langle 0110| + |1010\rangle\langle 1010| + |1100\rangle\langle 1100| + |0111\rangle\langle 0111| \\
&\quad + |1011\rangle\langle 1011| + |1101\rangle\langle 1101| + |1110\rangle\langle 1110| + |1111\rangle\langle 1111|
\end{aligned}$$

From these, with some work,

$$X \otimes I_{nf} = \frac{1}{2\sqrt{3}}(P_{13}P_{24} - P_{14}P_{23} + P_{14} + P_{23} - P_{13} - P_{24})$$

$$Z \otimes I_{nf} = \frac{1}{3}(P_{12}P_{34} - P_{12} - P_{34}) + \frac{1}{6}(P_{13} + P_{14} + P_{23} + P_{24} - P_{13}P_{24} - P_{14}P_{23}).$$

Again use the commutation relation to obtain

$$Y \otimes I_{nf} = \frac{1}{2i}[Z \otimes I_{nf}, X \otimes I_{nf}]$$

$$= \frac{i}{2}((X \otimes I_{nf})(Z \otimes I_{nf}) - (Z \otimes I_{nf})(X \otimes I_{nf})),$$

By using $P_{ij}P_{ij} = I$, $P_{ij}P_{kl}P_{ij} = P_{kl}$, $IP_{ij} = P_{ij}$, and trying to identify different permutation sequences that have the same effect, i.e. as was done for the $N = 3$ case, yields

$$Y \otimes I_{nf} = \frac{i}{4\sqrt{3}}(P_{34}P_{14} + P_{24}P_{12} + P_{13}P_{12} + P_{34}P_{23}$$

$$- P_{14}P_{34} - P_{12}P_{24} - P_{12}P_{13} - P_{23}P_{34}),$$

with the substitutions for equal operating tabulated at the end of the appendix. Thus for $N=4$ qubits the Pauli operators are

$$\begin{cases} X \otimes I_{nf} = \frac{1}{2\sqrt{3}}(P_{13}P_{24} - P_{14}P_{23} + P_{14} + P_{23} - P_{13} - P_{24}), \\ Y \otimes I_{nf} = \frac{i}{4\sqrt{3}}(P_{34}P_{14} + P_{24}P_{12} + P_{13}P_{12} + P_{34}P_{23} \\ \quad - P_{14}P_{34} - P_{12}P_{24} - P_{12}P_{13} - P_{23}P_{34}), \\ Z \otimes I_{nf} = \frac{1}{3}(P_{12}P_{34} - P_{12} - P_{34}) + \frac{1}{6}(P_{13} + P_{14} + P_{23} + P_{24} - P_{13}P_{24} - P_{14}P_{23}). \end{cases}$$

Moreover, expressed in Heisenberg interaction terms:

$$\begin{cases} X \otimes I_{nf} = \frac{1}{8\sqrt{3}}(\vec{\sigma}_1 \cdot \vec{\sigma}_4 + \vec{\sigma}_2 \cdot \vec{\sigma}_3 - \vec{\sigma}_1 \cdot \vec{\sigma}_3 - \vec{\sigma}_2 \cdot \vec{\sigma}_4 + (\vec{\sigma}_1 \times \vec{\sigma}_2) \cdot (\vec{\sigma}_3 \times \vec{\sigma}_4)), \\ Y \otimes I_{nf} = \frac{1}{8\sqrt{3}}(\vec{\sigma}_1 \cdot (\vec{\sigma}_3 \times \vec{\sigma}_4) + \vec{\sigma}_1 \cdot (\vec{\sigma}_2 \times \vec{\sigma}_3) - \vec{\sigma}_1 \cdot (\vec{\sigma}_2 \times \vec{\sigma}_4) - \vec{\sigma}_2 \cdot (\vec{\sigma}_3 \times \vec{\sigma}_4)), \\ Z \otimes I_{nf} = \frac{1}{24}(\vec{\sigma}_1 \cdot \vec{\sigma}_3 + \vec{\sigma}_1 \cdot \vec{\sigma}_4 + \vec{\sigma}_2 \cdot \vec{\sigma}_3 + \vec{\sigma}_2 \cdot \vec{\sigma}_4 + (\vec{\sigma}_1 \times \vec{\sigma}_2) \cdot (\vec{\sigma}_3 \times \vec{\sigma}_4)) \\ \quad - \frac{1}{12}(\vec{\sigma}_1 \cdot \vec{\sigma}_2 + \vec{\sigma}_3 \cdot \vec{\sigma}_4 + (\vec{\sigma}_1 \times \vec{\sigma}_4) \cdot (\vec{\sigma}_3 \times \vec{\sigma}_2)), \end{cases}$$

where the 4-spin interactions are described by the scalar quadruple product defined as

$$(\vec{\sigma}_i \times \vec{\sigma}_j) \cdot (\vec{\sigma}_k \times \vec{\sigma}_l) = (\vec{\sigma}_i \cdot \vec{\sigma}_k)(\vec{\sigma}_j \cdot \vec{\sigma}_l) - (\vec{\sigma}_i \cdot \vec{\sigma}_l)(\vec{\sigma}_j \cdot \vec{\sigma}_k) = \begin{vmatrix} \vec{\sigma}_i \cdot \vec{\sigma}_k & \vec{\sigma}_i \cdot \vec{\sigma}_l \\ \vec{\sigma}_j \cdot \vec{\sigma}_k & \vec{\sigma}_j \cdot \vec{\sigma}_l \end{vmatrix}$$

Table 1: Permutation equalities used

$P_{13}P_{12}$	$P_{12}P_{23}$
$P_{13}P_{14}$	$P_{34}P_{13}$
$P_{13}P_{23}$	$P_{12}P_{13}$
$P_{13}P_{34}$	$P_{12}P_{23}$
$P_{14}P_{12}$	$P_{12}P_{24}$
$P_{14}P_{13}$	$P_{34}P_{14}$
$P_{14}P_{24}$	$P_{12}P_{14}$
$P_{14}P_{34}$	$P_{34}P_{13}$
$P_{23}P_{12}$	$P_{12}P_{13}$
$P_{23}P_{13}$	$P_{12}P_{23}$
$P_{23}P_{24}$	$P_{34}P_{23}$
$P_{23}P_{34}$	$P_{24}P_{23}$
$P_{24}P_{12}$	$P_{12}P_{14}$
$P_{24}P_{14}$	$P_{12}P_{24}$
$P_{24}P_{23}$	$P_{34}P_{24}$
$P_{24}P_{34}$	$P_{34}P_{23}$
$P_{13}P_{12}P_{34}$	$P_{12}P_{34}P_{24}$
$P_{13}P_{14}P_{23}$	$P_{12}P_{34}P_{13}$
$P_{13}P_{24}P_{12}$	$P_{12}P_{14}P_{23}$
$P_{13}P_{24}P_{14}$	$P_{12}P_{34}P_{23}$
$P_{13}P_{24}P_{23}$	$P_{12}P_{34}P_{14}$
$P_{13}P_{24}P_{34}$	$P_{12}P_{13}P_{24}$
$P_{14}P_{12}P_{34}$	$P_{12}P_{34}P_{23}$
$P_{14}P_{13}P_{24}$	$P_{12}P_{34}P_{14}$
$P_{14}P_{23}P_{12}$	$P_{12}P_{13}P_{24}$
$P_{14}P_{23}P_{13}$	$P_{12}P_{34}P_{24}$
$P_{14}P_{23}P_{24}$	$P_{12}P_{34}P_{13}$
$P_{14}P_{23}P_{34}$	$P_{12}P_{14}P_{23}$
$P_{14}P_{34}P_{12}$	$P_{12}P_{34}P_{23}$
$P_{23}P_{12}P_{34}$	$P_{12}P_{34}P_{14}$
$P_{23}P_{13}P_{24}$	$P_{12}P_{34}P_{23}$
$P_{24}P_{12}P_{34}$	$P_{12}P_{34}P_{13}$
$P_{24}P_{14}P_{23}$	$P_{12}P_{34}P_{24}$
$P_{34}P_{13}P_{24}$	$P_{12}P_{14}P_{23}$
$P_{34}P_{14}P_{23}$	$P_{12}P_{13}P_{24}$
$P_{13}P_{24}P_{12}P_{34}$	$P_{14}P_{23}$
$P_{13}P_{24}P_{14}P_{23}$	$P_{12}P_{34}$
$P_{14}P_{23}P_{12}P_{34}$	$P_{13}P_{24}$
$P_{14}P_{23}P_{13}P_{24}$	$P_{12}P_{34}$