

Simple derivation of the Fong-Wandzura pulse sequence

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We give an analytic construction of a class of two-qubit gate pulse sequences that act on five of the six spin- $\frac{1}{2}$ particles used to encode a pair of exchange-only three-spin qubits. Within this class, the problem of gate construction reduces to that of finding a smaller sequence that acts on four spins and is subject to a simple constraint. The optimal sequence satisfying this constraint yields a two-qubit gate sequence equivalent to that found numerically by Fong and Wandzura. Our construction is sufficiently simple that it can be carried out entirely with pen, paper, and knowledge of a few basic facts about quantum spin.

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Controlled Heisenberg spin exchange is useful for realizing quantum gates in a quantum computer [1]. If qubits are encoded in the Hilbert space of one [1] or two [2] spin- $\frac{1}{2}$ particles, resources beyond exchange are required for universal quantum computation. Controlled exchange alone, however, is universal if qubits are encoded in the Hilbert space of at least three spin- $\frac{1}{2}$ particles [3–5].

Semiconductor quantum dots with trapped electrons are promising systems for manipulating spin-1/2 particles [6]. Controlled exchange between pairs of electron spins in quantum dots has been demonstrated [7] and used to manipulate a variety of three-spin encoded qubits [8–13], including the resonant exchange qubit [14–16] which maintains encoding by keeping the intraqubit exchange “always on” (see also [17]). Here we assume the exchange is kept off except when pulsed, i.e., adiabatically switched on and off, between pairs of spins. It is then necessary to design pulse sequences that realize quantum gates on encoded qubits without resulting in leakage out of the encoded space [5,11,18–22].

Designing such sequences is straightforward for single-qubit gates but poorly understood for two-qubit gates. The difficulty comes from the no-leakage constraint combined with the large search space of operators acting on six spins. Not surprisingly, the shortest known two-qubit gate sequence, presented by Fong and Wandzura [20], was found by a numerical search which offers little insight into its derivation. Furthermore, existing analytic derivations of less optimal sequences are lengthy and complicated [19,22].

In this Rapid Communication we analytically construct a class of pulse sequences for two-qubit gates. We show that within this class the most efficient sequence is equivalent to the Fong-Wandzura sequence. Throughout our construction we avoid as much as possible complicated calculations and use only the most basic facts about quantum spin [23].

Because we exclusively consider rotationally invariant operators we are free to describe states of multiple spins using only total spin quantum numbers. Accordingly, we employ the notation of [22] where each spin- $\frac{1}{2}$ is represented by the symbol \bullet and groups of spins are enclosed in ovals labeled by total spin. Figure 1(a) shows the encoding of [5] in which qubits are stored in the Hilbert space of three spin- $\frac{1}{2}$ particles with a total spin of $\frac{1}{2}$ in this notation. In the text we write these states using parentheses instead of ovals. The qubit states of Fig. 1(a) defining the computational basis are then $(\bullet(\bullet\bullet)_a)_{1/2} = |a\rangle$ with $a = 0$ and 1, for which the two rightmost spins form a

singlet and triplet, respectively. Leakage out of the encoded space then involves transitions to the noncomputational state $(\bullet\bullet\bullet)_{3/2}$. Figure 1(b) shows six spins encoding two qubits and highlights the five spins the pulse sequences we consider act on, where the total spin f can be either $\frac{1}{2}$ or $\frac{3}{2}$.

Consider the exchange Hamiltonian $H = J\mathbf{S}_i \cdot \mathbf{S}_j$ acting on two spins $(\bullet\bullet)_a$ whose Hilbert space is spanned by the two states with total spin $a = 0$ and 1. (Because only total spin quantum numbers are relevant, we treat the three-fold degenerate $a = 1$ state as a single state.) Pulsing this Hamiltonian for a duration t measured in units of π/J results in the time evolution operator (up to an irrelevant overall phase factor)

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

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 $2 - t$.

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, equivalent to physically exchanging two spins [24]. Figure 2(a) shows an r pulse acting on the state $(\bullet\bullet)_a$ using standard notation with pulses represented by double arrows labeled by duration. The corresponding matrix representation of the resulting operation, also given in Fig. 2(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 -1 for $r = 0$ or 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) and two explicit SWAPS is shown in Fig. 2(b). For $r = 0$ the two SWAPS square to the identity. For $r = 1$ the sequence consists of five SWAPS which, when viewed as spin permutations, are readily seen to be equivalent to a single SWAP acting on the top two spins. In both cases, the effect of the sequence is to multiply the state $((\bullet\bullet)_a(\bullet\bullet)_b)_c$ by 1 if $a = 0$, and m if $a = 1$, regardless of the value of c , where, as in Fig. 2(a), $m = 1$ or -1 for $r = 0$ or 1, respectively. The corresponding matrix representation is also given in Fig. 2(b).

We seek pulse sequences which act on the five spins $((\bullet\bullet)_a(\bullet\bullet)_b)_{1/2}_f$ highlighted in Fig. 1(b) and carry out leakage-free two-qubit gates. We refer to the qubits with state

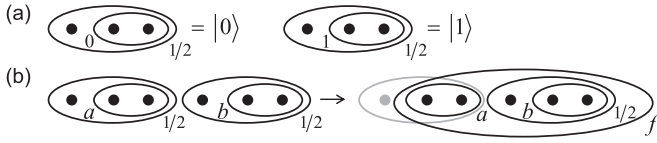


FIG. 1. (a) Three-spin qubit encoding. (b) Two qubits in states a and b and a diagram highlighting the five rightmost spins with total spin $f = \frac{1}{2}$ or $\frac{3}{2}$.

labels a and b as the control and target qubit, respectively. Our construction is based on using a smaller sequence which acts on the four rightmost spins in Fig. 1(b) and carries out an operation we denote R which, as seen shortly, is closely related to an r pulse. One requirement we place on 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- $\frac{1}{2}$ particle,

$$(\bullet(\bullet\bullet)_b)_{1/2} \rightarrow \star. \quad (2)$$

Matrix elements of operations acting on any collection of spins including \star are then elevated from numbers to 2×2 blocks that act on the Hilbert space of the target qubit hidden within \star .

We require that when R is applied to the state $(\bullet\star)_d$ 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. 3(a). Such R operations can be viewed as generalized r pulses where the matrix elements 1 and m , with $m^2 = 1$, of Fig. 2(a) have been elevated to the 2×2 matrices $\mathbb{1}$ and M , with $M^2 = \mathbb{1}$ in Fig. 3(a).

This view of R as an elevated r pulse suggests the five-pulse sequence of Fig. 2(b) can also be elevated to the sequence shown in Fig. 3(b). This sequence acts on the effective Hilbert space spanned by the states $((\bullet\bullet)_a\star)_f$ with $af = 0\frac{1}{2}, 1\frac{1}{2}$, and $1\frac{3}{2}$ and consists of three R operations and two SWAPS. The only 2×2 block element in the matrix representation of R not proportional to the identity is M . Because $M^2 = \mathbb{1}$, when evaluating the matrix representation for the full sequence, each

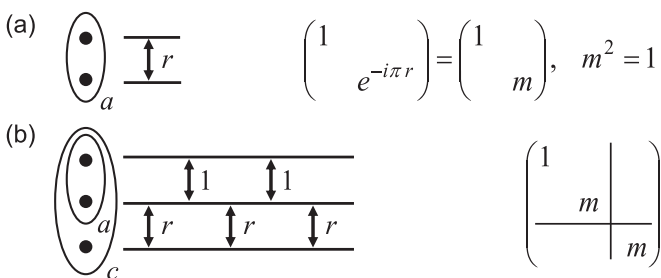


FIG. 2. (a) Elementary exchange pulse of duration $r = 0$ or 1 , referred to as an r pulse in the text, and matrix representation of the resulting operation in the basis $a = \{0, 1\}$, where $m = 1$ or -1 for $r = 0$ or 1 , respectively. (b) Sequence of three r pulses and two explicit SWAPS (r pulses with $r = 1$) acting on three spins and the matrix representation of the resulting operation in the basis $ac = \{0\frac{1}{2}, 1\frac{1}{2} | 1\frac{3}{2}\}$.

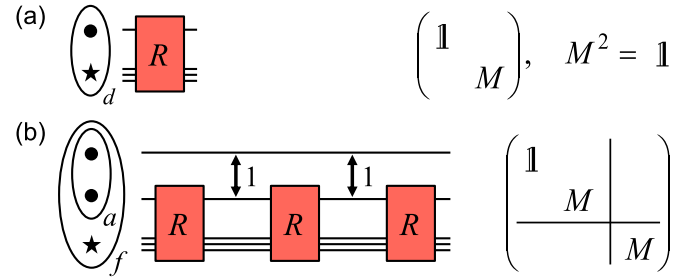


FIG. 3. (a) R operation acting on a spin- $\frac{1}{2}$ particle, \bullet , and an effective spin- $\frac{1}{2}$ particle, \star , defined in Eq. (2). The matrix representation of this operation is given in the effective basis $d = \{0, 1\}$ where $\mathbb{1}$ is the 2×2 identity, and M is a 2×2 matrix where $M^2 = \mathbb{1}$, both of which act on the target qubit hidden within \star . (b) Pulse sequence generalizing that shown in Fig. 2(b). The matrix representation of the resulting operation is given in the effective basis $af = \{0\frac{1}{2}, 1\frac{1}{2} | 1\frac{3}{2}\}$.

block matrix element must be of the form $\alpha_0 \mathbb{1} + \alpha_1 M$. The coefficients α_0 and α_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(b). It follows that the matrix representation of the operation carried out by this sequence in the effective $af = \{0\frac{1}{2}, 1\frac{1}{2} | 1\frac{3}{2}\}$ basis is that given in Fig. 3(b), i.e., an elevated version of the matrix shown in Fig. 2(b). To prove this we only used the fact that $M^2 = \mathbb{1}$. It therefore holds not just for $M = \pm \mathbb{1}$, but also for $M = \hat{\mathbf{n}} \cdot \boldsymbol{\sigma}$ where $\hat{\mathbf{n}}$ is any real-valued unit vector and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the Pauli vector.

The pulse sequence shown in Fig. 3(b) acting on the two qubits of Fig. 1(b) 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

$$U_{2\text{qubit}} = \text{diag}(\mathbb{1}, M). \quad (3)$$

For $M = \pm \mathbb{1}$ the resulting gate is not entangling. However, for $M = \hat{\mathbf{n}} \cdot \boldsymbol{\sigma}$ the sequence enacts a leakage-free controlled- $(\hat{\mathbf{n}} \cdot \boldsymbol{\sigma})$ gate which is equivalent to a controlled-NOT (CNOT) gate (for which $\hat{\mathbf{n}} = \hat{\mathbf{x}}$), up to single-qubit rotations.

Abandoning the notation \star we now consider R acting on the four-spin Hilbert space spanned by the states $(\bullet((\bullet\bullet)_b\bullet)_c)_d$ where, since c is initially $\frac{1}{2}$, d is either 0 or 1. The requirements on R are then that it must (i) preserve the quantum number c , and (ii) in the restricted Hilbert space with $c = \frac{1}{2}$, have the form shown in Fig. 3(a) with $M = \hat{\mathbf{n}} \cdot \boldsymbol{\sigma}$.

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

$$\langle\langle(\bullet\bullet)_1(\bullet\bullet)_1|_1|V|(\bullet\bullet\bullet\bullet)_{3/2}|_1\rangle\rangle = 0 \quad (4)$$

depicted in Fig. 4(a). As shown below, inserting any V satisfying Eq. (4) into the sequence shown in Fig. 4(b) results in an R operation with $M = \hat{\mathbf{n}} \cdot \boldsymbol{\sigma}$. Letting $U_{ij}(t)$ denote an exchange pulse of duration t acting on spins i and j , as defined in Eq. (1), the sequence for R can be written $V^{-1}U_{12}(1)U_{34}(1)V$, using the spin labeling of Fig. 4(b). From Eq. (1), the matrix representation of the two SWAPS

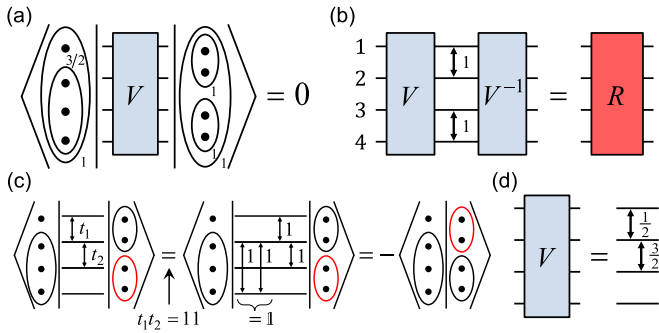


FIG. 4. (a) Constraint which must be satisfied by an operation V used in our construction. (b) Sequence in which V , its inverse, and two SWAPs carry out an R operation. (c) Evaluation of the matrix element (6) for the case $t_1 t_2 = 11$, as described in the text. [Quantum numbers omitted for readability are as in (a).] (d) Two-pulse solution of (a) for V .

$U_{12}(1)U_{34}(1)$ in the $((\bullet\bullet)_b(\bullet\bullet)_d)$ basis with state ordering $bb'd = \{000, 110|011, 101, 111\}$ is

$$U_{12}(1)U_{34}(1) = \text{diag}(1, 1| -1, -1, 1). \quad (5)$$

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. For $d = 1$, Eq. (4) implies V maps the $c = \frac{3}{2}$ state $(\bullet(\bullet\bullet\bullet)_{3/2})_1$ entirely into the $b'b = 01, 10$ subspace. The two SWAPs 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 is to multiply the $c = \frac{3}{2}$ state by -1 . The fact that R maps the $c = \frac{3}{2}$ state onto itself implies that R also maps the $c = \frac{1}{2}$ 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. (5)], the trace of the full sequence $V^{-1}U_{12}(1)U_{34}(1)V$ in this sector is also -1 . Thus, since the $c = \frac{3}{2}$ matrix element of the full sequence is -1 , the trace of the operation acting on the $c = \frac{1}{2}$ subspace must be 0. Finally, because the two SWAPs $U_{12}(1)U_{34}(1)$ square to the identity, the full sequence for R squares to the identity. The operation carried out by this sequence on the $c = \frac{1}{2}$ subspace in the $d = 1$ sector must therefore also square to the identity and, because it is traceless, must have the form $M = \hat{n} \cdot \sigma$.

The set of pulse sequences V that satisfy the constraint (4) can be used to construct 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 Eq. (4) is 2 and for this optimal case the resulting two-qubit gate sequence is equivalent to the Fong-Wandzura sequence.

Without loss of generality we take $V = U_{23}(t_2)U_{12}(t_1)$. To determine t_1 and t_2 for which V satisfies Eq. (4) we employ a simple ‘‘pen and paper’’ procedure based on the observation that Eq. (1) implies

$$\begin{aligned} & \langle ((\bullet\bullet)_1(\bullet\bullet)_1)_1 | U_{23}(t_2)U_{12}(t_1) | (\bullet(\bullet\bullet\bullet)_{3/2})_1 \rangle \\ & = \alpha + \beta e^{-i\pi t_1} + \gamma e^{-i\pi t_2} + \delta e^{-i\pi(t_1+t_2)}, \end{aligned} \quad (6)$$

where the coefficients α, β, γ , and δ can be found by evaluating the four cases $t_1 t_2 = 00, 01, 10$, and 11 . For $t_1 t_2 = 00$ the left-hand side of Eq. (6) is simply equal to $F \equiv \langle ((\bullet\bullet)_1(\bullet\bullet)_1)_1 | (\bullet(\bullet\bullet\bullet)_{3/2})_1 \rangle$ [25]. For $t_1 t_2 = 01$ and 10 there

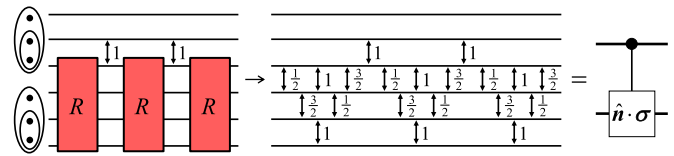


FIG. 5. Sequence of Fig. 3(b) acting on two encoded qubits resulting in a controlled- $(\hat{n} \cdot \sigma)$ gate. Also shown is the full sequence obtained by first inserting the optimal sequence for V from Fig. 4(d) into the sequence for R from Fig. 4(b) and inserting the result into the sequence from Fig. 3(b). This sequence is equivalent to the Fong-Wandzura sequence.

is a single SWAP which can be applied either to the left (for $t_1 t_2 = 01$) or right (for $t_1 t_2 = 10$) four-spin state in Fig. 4(a). Since each SWAP then acts on a pair of spins with total spin 1, the result is an overall factor of -1 using the phase convention of Eq. (1). In both cases the matrix element (6) is thus equal to $-F$.

For the remaining case $t_1 t_2 = 11$ both pulses are SWAPs and a method for evaluating Eq. (6) is sketched in Fig. 4(c). First, a pair of SWAPs which combine to the identity $U_{24}(1)U_{24}(1) = \mathbb{1}$, is inserted at the start of the sequence. We then view the four SWAPs as physical particle exchanges. It is irrelevant that particle exchange differs from SWAP by a factor of -1 because there are an even number of SWAPs. Applying one of the exchanges of spins 2 and 4 to the state $(\bullet(\bullet\bullet\bullet)_{3/2})_1$ then gives a factor $+1$, since the two exchanged spins have total spin 1. The remaining three exchanges can then be applied to the state $((\bullet\bullet)_1(\bullet\bullet)_1)_1$ where, referring to Fig. 4(c), they result in a permutation which exchanges the bottom two spins (red oval) with the top two spins (black oval). This exchange of two spin-1 objects with total spin 1 results in a factor of -1 . Thus the $t_1 t_2 = 11$ matrix element (6) is equal to $-F$.

Having evaluated the left-hand side of Eq. (6) for the four cases $t_1 t_2 = 00, 01, 10$, 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. (4), $t_1 t_2 = \frac{1}{2}, \frac{3}{2}, \frac{3}{2}, \frac{1}{2}$. Figure 4(d) shows the resulting sequence for the first solution, which consists of one $\sqrt{\text{SWAP}}(t = \frac{1}{2})$ and one inverse $\sqrt{\text{SWAP}}(t = \frac{3}{2})$.

Figure 5 shows the pulse sequence obtained by inserting the sequence for V from Fig. 4(d) into Fig. 4(b) and inserting the resulting sequence for R into Fig. 3(b). This sequence can be applied to a linear array of spins with nearest-neighbor pulses and carries out a controlled- $(\hat{n} \cdot \sigma)$ gate consisting of eight SWAPs, six $\sqrt{\text{SWAP}}$ s, and six inverse $\sqrt{\text{SWAP}}$ s [26]. After removing single-qubit rotations, the core Fong-Wandzura sequence as published in [20] consists of six SWAPs, three $\sqrt{\text{SWAP}}$ s, and nine inverse $\sqrt{\text{SWAP}}$ s. Our sequence can be converted into the Fong-Wandzura sequence using elementary manipulations in which pairs of SWAPs are inserted [as in Fig. 4(c)] or removed, and single SWAPs are pulled past other pulses and in some cases combined with $\sqrt{\text{SWAP}}$ s to form inverse $\sqrt{\text{SWAP}}$ s (and vice versa). The same manipulations can be used to produce sequences applicable to spin geometries other than linear [21]. These manipulations preserve the number of nontrivial (i.e., not SWAP) pulses in these sequences as well as the parity of the sum of the number of SWAPs and

$\sqrt{\text{SWAP}}$ s. This parity is odd for the Fong-Wandzura sequence and even for our construction, consistent with the fact that a single-qubit operation corresponding to a single SWAP must be added to the core Fong-Wandzura sequence to produce a controlled- $(\hat{\mathbf{n}} \cdot \boldsymbol{\sigma})$ gate.

In summary, we have analytically constructed a class of two-qubit gate pulse sequences for exchange-only quantum computation. These sequences are elevated versions of the simple three-spin sequences shown in Fig. 2(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 (4). 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.

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 [23] The essential ingredients in our construction are the familiar spin addition rule, $s_1 \otimes s_2 = |s_1 - s_2|, |s_1 - s_2| + 1, \dots, s_1 + s_2$, and the fact that interchanging two spin- s particles with total spin S_{tot} results in a factor of $(-1)^{2s - S_{\text{tot}}}$.
 [24] For the phase choice in Eq. (1) a SWAP is equivalent to exchanging particles and multiplying the result by -1 .
 [25] Direct calculations gives $F = 1/\sqrt{3}$, up to a phase factor equal to 1 for the Condon-Shortley convention.
 [26] For the sequence in Fig. 4(d), $\hat{\mathbf{n}} = (0, \sqrt{3}/2, -1/2)$ with the direction of the xy component fixed by the Condon-Shortley convention.