

Realization of controlled NOT quantum gate via control of a two spin system

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Abstract. Physical realization of controlled NOT quantum gate is addressed as a control problem for the system of two interacting spins. The control is carried out by magnetic pulses acting on the spins. The shapes of the appropriate magnetic pulses are computed.

Key words: quantum gates control, CNOT gate, quantum control.

1. Introduction

Quantum mechanics can be used to process information [1–4]. The unit of quantum information is called a *qubit* (quantum bit), quantum counterpart of the classical bit. Physically, qubit is a two level quantum system. There are many examples of such systems, e.g., horizontal and vertical polarization of photon, two states of the half spin particle, or two chosen states of an atom (denoted as ground state and excited state).

In the paper the problem of quantum CNOT gate is addressed. The problem is casted as a control task, and is a particular example of a quantum control problem. Quantum control theory undergoes rapid development and is of interest to different communities ranging from physics, applied mathematics, chemistry, and quantum computing [5]. There is a plethora of applications of quantum control, mainly in physics and chemistry, an interested reader is referred to many books and survey papers, e.g., [6–15]. One of the key issues in classical control theory is controllability of the system under consideration, the quantum systems are not exception in this regard. One is interested, whether a quantum system can be driven to a desired state, by an appropriate control input. The practical importance of this problem is clearly made apparent by, e.g., [16–18]. However, many definitions of the quantum system controllability have been proposed, among them, pure state controllability, complete controllability, eigenstate controllability and kinematic controllability [16–22]. The major contribution of this paper is demonstration, that in the particular case of CNOT gate realized as a system of two interacting spins, the control can be relatively easy computed numerically, by a simple trial and failure method. Although the case is particular it is of importance since CNOT gate enables quantum entanglement generation [1–4].

The paper is organized as follows. Section 2 introduces, mainly for further reference, some basic notions, such as quantum states, quantum bit (qubit), or Bloch sphere. Section 3 contains the preliminaries such as quantum measurements, quantum entanglement, quantum gates and the link between binary quantum gates and entanglement generation. Section 4

discusses the realization of CNOT gate as a system of two interacting spins controlled by magnetic pulses. The Subsec. 4.1 recapitulates results already known from the literature [4]. The Subsec. 4.1 is, to the best knowledge of authors, the original contribution of the paper. It generalizes the results of Subsec. 4.1 onto the case of time-dependent Hamiltonian and time-varying pulses (in contrast to the constant values of magnetic field applied to the time-independent Hamiltonian case discussed in Subsec. 4.1). The Subsec. 4.3 contains the results of the numerical computations and simulations involving the computed magnetic pulses).

2. Notation

Throughout the paper we use standard Dirac notation [23], for more information on the concepts and notions presented in this section one is referred to, e.g., [1, 3, 4].

2.1. Qubit. A classical bit is a system which can assume two different states, representing 0 and 1. The only operations that can be done on that system are identity ($0 \mapsto 0$, $1 \mapsto 1$) and negation NOT ($0 \mapsto 1$, $1 \mapsto 0$). A quantum bit, *qubit* is a two level quantum system, described by two dimensional complex Hilbert space. Two mutually orthogonal vectors from that space

$$|0\rangle \equiv \begin{bmatrix} 1 & 0 \end{bmatrix}^T, \quad |1\rangle \equiv \begin{bmatrix} 0 & 1 \end{bmatrix}^T \quad (1)$$

can be used to represent the values 0 and 1 of a classical bit. The two states (1) constitute a computational basis.

State vectors are defined up to global phase factor (which has no physical meaning), thus, making use of the superposition principle, one can write a general state of the qubit in the following form

$$|\psi\rangle = \cos \frac{\theta}{2} |0\rangle + e^{i\varphi} \sin \frac{\theta}{2} |1\rangle, \quad (2)$$

where θ and φ are real parameters, $0 \leq \theta \leq \pi$, $0 \leq \varphi < 2\pi$. From (2), one can see that there exist infinitely many states of a qubit, in fact, their set is of the continuum cardinality.

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According to [3], a two level quantum system can be used as a qubit if it satisfies the following conditions:

1. It can be prepared in an desired, uniquely defined state, e.g., $|0\rangle$.
2. An arbitrary state of the qubit can be transformed to an arbitrary other state by unitary transformation.
3. The state of the qubit can be measured in computational basis $\{|0\rangle, |1\rangle\}$, i.e., it is possible to measure a qubit along the z direction. The Pauli \hat{Z} operator corresponds to this measurement, it has the eigenstates $|0\rangle$ and $|1\rangle$. The measurement result of the qubit in the state (2) is 0 or 1, with the probability, respectively,

$$\begin{aligned} p_0 &= |\langle 0|\psi\rangle|^2 = \cos^2 \frac{\theta}{2}, \\ p_1 &= |\langle 1|\psi\rangle|^2 = \sin^2 \frac{\theta}{2}. \end{aligned} \quad (3)$$

2.2. Bloch sphere and Bloch vector. The state of the qubit (2) can be represented by a point on the sphere of unit radius, the so called Bloch sphere, thus any given state of a qubit can be represented by a unitary Bloch vector. The Bloch vector can be defined in the spherical coordinates, if this is the case, the Bloch vector corresponding to the state (2) is given by zenithal angle θ and azimuthal angle φ . The Bloch vector can also be given by his x, y, z coordinates in the \mathbb{R}^3 space (in which the Bloch sphere is submerged), then $x = \sin \theta \cos \varphi$, $y = \sin \theta \sin \varphi$, $z = \cos \theta$.

3. Preliminaries

3.1. Qubit state measurement. The state $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ of a qubit can be measured up to the arbitrary precision, assuming an appropriate number of the qubits prepared in this state is available. See, e.g., [3] for more details.

3.2. Two qubit states and quantum entanglement. A system composed of two subsystems, each being a qubit, is described by tensor product of two qubits. If the Hilbert space \mathcal{H}_1 is associated with subsystem 1 and the Hilbert space \mathcal{H}_2 is associated with subsystem 2, then the space $\mathcal{H}_1 \otimes \mathcal{H}_2$ corresponds to the composite system.

The standard basis for a two qubit system is $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$, and the following convention is used

$$|ab\rangle \equiv |a\rangle|b\rangle \equiv |a\rangle \otimes |b\rangle.$$

The generalization of the above reasoning onto the multi qubit systems is straightforward.

Quantum entanglement, one of the most interesting phenomena in quantum mechanics, can be observed already for two qubit states. Consider the space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ which is tensor product of \mathcal{H}_1 and \mathcal{H}_2 , as well as appropriate states belonging to these spaces $|\psi\rangle \in \mathcal{H}$, $|\alpha\rangle \in \mathcal{H}_1$, $|\beta\rangle \in \mathcal{H}_2$. Taking into account that a standard basis of the space \mathcal{H} is $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$, whereas the standard basis for the space \mathcal{H}_1 and \mathcal{H}_2 is $\{|0\rangle, |1\rangle\}$, one can write

$$\begin{aligned} |\psi\rangle &= \psi_1|00\rangle + \psi_2|01\rangle + \psi_3|10\rangle + \psi_4|11\rangle, \\ |\alpha\rangle &= \alpha_1|0\rangle + \alpha_2|1\rangle, \quad |\beta\rangle = \beta_1|0\rangle + \beta_2|1\rangle. \end{aligned}$$

Not every state $|\psi\rangle \in \mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ can be written as a tensor product of the states $|\alpha\rangle \in \mathcal{H}_1$ and $|\beta\rangle \in \mathcal{H}_2$

$$|\psi\rangle = |\alpha\rangle \otimes |\beta\rangle = (\alpha_0|0\rangle + \alpha_1|1\rangle) \otimes (\beta_0|0\rangle + \beta_1|1\rangle). \quad (4)$$

The states $|\psi\rangle \in \mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ that cannot be written in the form of the tensor product (4), are called *entangled* (in contrast to the *separable* states). Quantum entanglement does not have an analogue in classical physics.

3.3. Unary quantum gates. Unary gates operate on single qubits. Operations on a qubit must preserve normalization of its state, thus they are described by unitary matrices of size 2×2 . One can show that all these operations can be realized with use of two gates, i.e., the Hadamard gate and phase-shift gate [1, 3].

The \hat{X} , \hat{Y} and \hat{Z} gates are defined as $\hat{X}|a\rangle = |1 \oplus a\rangle$, $\hat{Y}|a\rangle = i(-1)^a|1 \oplus a\rangle$, $\hat{Z}|a\rangle = (-1)^a|a\rangle$, where $a \in \{0, 1\}$, and \oplus denotes modulo 2 addition, thus $\hat{X}(\alpha|0\rangle + \beta|1\rangle) = \alpha|1\rangle + \beta|0\rangle$, $\hat{Y}(\alpha|0\rangle + \beta|1\rangle) = -i(\beta|0\rangle - \alpha|1\rangle)$ and $\hat{Z}(\alpha|0\rangle + \beta|1\rangle) = \alpha|0\rangle - \beta|1\rangle$. In the basis $\{|0\rangle, |1\rangle\}$ the gates are given by the matrices

$$\hat{X} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \hat{Y} = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \hat{Z} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

The **Hadamard gate** is defined as $\hat{H}|a\rangle = \frac{1}{\sqrt{2}}((-1)^a|a\rangle + |1 \oplus a\rangle)$ where $a \in \{0, 1\}$. \hat{H} is hermitian, $\hat{H}^2 = \hat{I}$ and $\hat{H}^{-1} = \hat{H}$. In the basis $\{|0\rangle, |1\rangle\}$ the gate is given by the matrix

$$\hat{H} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}. \quad (5)$$

The **Phase-shift gate** is defined as $\hat{R}_z(\delta)|a\rangle = e^{ia\delta}|a\rangle$ where $a \in \{0, 1\}$. Since $\hat{R}_z(\delta)|0\rangle = |0\rangle$ and $\hat{R}_z(\delta)|1\rangle = e^{i\delta}|1\rangle$, the states of the basis, up to the global phase, do not change, however, the state of the qubit as a whole changes, since the mutual phase changes. Taking into account the parametrization (2), which is more natural when one considers a qubit as a point on the Bloch sphere, one has

$$\hat{R}_z(\delta)|\psi\rangle = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\delta} \end{bmatrix} \begin{bmatrix} \cos \frac{\theta}{2} \\ e^{i\varphi} \sin \frac{\theta}{2} \end{bmatrix} = \begin{bmatrix} \cos \frac{\theta}{2} \\ e^{i(\varphi+\delta)} \sin \frac{\theta}{2} \end{bmatrix}. \quad (6)$$

The phase-shift gate corresponds to the rotation, counterclockwise, by the δ angle, around z axis on the Bloch sphere.

A unitary operation on the state of the qubit corresponds to the rotation of the Bloch vector of the qubit on the Bloch sphere. Any such a transformation (i.e., any rotation of the Bloch sphere) can be realized with Hadamard gates and phase-shift gates, for more details one is referred to, e.g., [3].

3.4. Binary gates and entanglement generation. The interaction of spins is the source of entanglement, thus in order to prepare an entangled state one has to use a binary gate. In particular, the controlled not gate (CNOT gate) is a binary gate which can be used for entanglement generation. The CNOT gate acts on the states of computational basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$ similarly to the classical XOR gate: $\text{CNOT}(|x\rangle|y\rangle) = |x\rangle|x \oplus y\rangle$, where $x, y \in \{0, 1\}$, and \oplus , as already mentioned, denotes addition modulo 2. The first input qubit is called the control qubit, the second one is called the target qubit. The gate changes the target qubit if the control qubit is equal to 1, otherwise the target qubit remains unchanged. The matrix representation of the CNOT gate in the basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$ has the form

$$\text{CNOT} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}. \quad (7)$$

Using CNOT gate, one can generate entangled states, in particular the Bell states [3].

4. Realization of the CNOT gate via two interacting spins

The CNOT gate acts on the two qubit state in the following way

$$\text{CNOT}(|a\rangle|b\rangle) = |a\rangle|a \oplus b\rangle, \quad a, b \in \{0, 1\}.$$

The CNOT gate can be realized with use of the Hadamard gates \hat{H} and \hat{C}_Z gates, where \hat{C}_Z is the so called controlled \hat{Z} gate, defined in the following way

$$\hat{C}_Z|a\rangle|b\rangle = |a\rangle((1 \oplus a)|b\rangle + a\hat{Z}|b\rangle),$$

where $\hat{Z}|a\rangle = (-1)^a|a\rangle$. One has

$$\begin{aligned} \text{CNOT} &= \frac{1}{2}(\hat{I} \otimes \hat{I} + \hat{Z} \otimes \hat{I} + \hat{I} \otimes \hat{H}\hat{Z}\hat{H} - \hat{Z} \otimes \hat{H}\hat{Z}\hat{H}) \\ &= (\hat{I} \otimes \hat{H}) \hat{C}_Z (\hat{I} \otimes \hat{H}), \end{aligned} \quad (8)$$

where

$$\hat{C}_Z = \frac{1}{2}(\hat{I} \otimes \hat{I} + \hat{I} \otimes \hat{Z} + \hat{Z} \otimes \hat{I} - \hat{Z} \otimes \hat{Z}).$$

Denoting $\hat{H}_0 \equiv \hat{I} \otimes \hat{H}$, $\hat{Z}_0 \equiv \hat{I} \otimes \hat{Z}$, $\hat{Z}_1 \equiv \hat{Z} \otimes \hat{I}$, one can write

$$\hat{C}_Z = \frac{1}{2}(\hat{I} + \hat{Z}_0 + \hat{Z}_1 - \hat{Z}_1\hat{Z}_0) \quad (9)$$

and

$$\text{CNOT} = \hat{H}_0 \hat{C}_Z \hat{H}_0. \quad (10)$$

Taking into account (9) and (10) one can state that the realization of the CNOT gate reduces to the realization of \hat{C}_Z (up to the Hadamard operation). Since $\hat{C}_Z^2 = \hat{I}$ one can write

$$e^{i\theta\hat{C}_Z} = \hat{I} \cos \theta + i\hat{C}_Z \sin \theta. \quad (11)$$

Substituting $\theta = \frac{\pi}{2}$ in (11) yields

$$\begin{aligned} \hat{C}_Z &= -ie^{i\frac{\pi}{2}\hat{C}_Z} = -ie^{i\frac{\pi}{4}(\hat{I} + \hat{Z}_1 + \hat{Z}_0 - \hat{Z}_1\hat{Z}_0)} \\ &= e^{-i\frac{\pi}{4}} e^{i\frac{\pi}{4}(\hat{Z}_1 + \hat{Z}_0 - \hat{Z}_1\hat{Z}_0)}. \end{aligned}$$

A quantum system described by Hamiltonian \mathcal{H} evolves according to the Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \mathcal{H}(t) |\psi(t)\rangle. \quad (12)$$

This evolution in the period of time $[0, \tau]$ corresponds to the transformation $|\psi(0)\rangle \mapsto |\psi(\tau)\rangle$. To realize a gate \hat{C}_Z , for which $|00\rangle = \hat{C}_Z|00\rangle$, $|01\rangle = \hat{C}_Z|01\rangle$, $|10\rangle = \hat{C}_Z|10\rangle$, $-|11\rangle = \hat{C}_Z|11\rangle$, one has to choose Hamiltonian \mathcal{H} in (12) in such a way, an initial state $|\psi(0)\rangle$ equal to, respectively $|00\rangle, |01\rangle, |10\rangle, |11\rangle$ results in a final state $|\psi(\tau)\rangle$, equal to, respectively $|00\rangle, |01\rangle, |10\rangle, -|11\rangle$, respectively. The problem discussed is a special case of the more general scheme, the so called bilinear model [5]. Rewriting (12) as

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \left[\mathcal{H}_0 + \sum_k u_k(t) \mathcal{H}_k \right] |\psi(t)\rangle, \quad (13)$$

as can readily be seen, the control of the system is exerted by a set of functions $u_k(t)$, driving the system from the initial state $|\psi_0\rangle$ into the final state $|\psi_f\rangle$. The total Hamiltonian of the system

$$\mathcal{H} = \mathcal{H}_0 + \sum_k u_k(t) \mathcal{H}_k,$$

completely determines the controlled evolution of the system. The operators \mathcal{H}_k , ($k = 1, 2, \dots$) are called interaction Hamiltonians.

For the time independent Hamiltonian one can give an explicit solution of the Eq. (12), the case of time dependent Hamiltonian is more complicated. Thus, first the time-independent case will be considered and then the time dependent one.

4.1. Time independent Hamiltonian. The following analysis derives from [4] (indirectly from [24]). The solution of the Eq. (12) for the time independent Hamiltonian reads:

$$|\psi(t)\rangle = e^{-\frac{i\mathcal{H}t}{\hbar}} |\psi(0)\rangle.$$

From now on we assume $\hbar = 1$. There is a unitary transformation, which transforms the input state (the initial state) $|\psi(0)\rangle$ (within the time period $[0, \tau]$) into the output (final) state $|\psi(\tau)\rangle$, thus, to realize the gate \hat{C}_Z one has to choose the Hamiltonian \mathcal{H} satisfying, up to a global factor ϕ , the equation

$$\hat{C}_Z = e^{i\phi} e^{-i\mathcal{H}\tau}.$$

The gate is realized via a system of two interacting spins and the Hamiltonian \mathcal{H} describes the interaction of the exogenous magnetic fields on the qubits (spins) of the system, as well as mutual interactions between the qubits (spins).

It will be shown that the gate \hat{C}_Z can be realized, up to global phase factor, via the interaction of two qubits described by the Hamiltonian proportional to $\hat{Z}_1 + \hat{Z}_0 - \hat{Z}_1\hat{Z}_0$, within an appropriately chosen time period $[0, \tau]$.

The so called exchange interaction is a natural interaction between two spins is given by

$$\begin{aligned}\vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(0)} &\equiv (\hat{X}_1 \hat{X}_0 + \hat{Y}_1 \hat{Y}_0 + \hat{Z}_1 \hat{Z}_0) \\ &\equiv (\hat{X} \otimes \hat{X} + \hat{Y} \otimes \hat{Y} + \hat{Z} \otimes \hat{Z}).\end{aligned}$$

The gate \hat{C}_Z can be implemented with two spins $\vec{\sigma}^{(1)}$ and $\vec{\sigma}^{(0)}$ subjected to appropriately chosen magnetic fields. For the Hamiltonian

$$\mathcal{H} = \mathcal{J} \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(0)} + B_1 \hat{Z}_1 + B_0 \hat{Z}_0, \quad (14)$$

one wants to realize, up to the global phase, the gate

$$\hat{C}_Z = e^{-i\mathcal{H}\tau},$$

by an appropriate choice of \mathcal{J} (the so called coupling constant), B_1 , B_0 (magnetic fields acting on spins), and the evolution time τ . More precisely, B_0 and B_1 appearing in (14) are not the magnetic fields but are proportional to them, the proportionality coefficients are, μ_0 and μ_1 , i.e., the magnetic moments of spins. To simplify the notation we will call B_0 and B_1 shortly magnetic fields.

Denoting $B_+ \equiv B_1 + B_0$, $B_- \equiv B_1 - B_0$, we obtain

$$\mathcal{H} = \mathcal{J} \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(0)} + \frac{1}{2} B_+ (\hat{Z}_1 + \hat{Z}_0) + \frac{1}{2} B_- (\hat{Z}_1 - \hat{Z}_0). \quad (15)$$

where the Hamiltonian (15) consists of three terms, the first term is proportional to $\vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(0)}$, the second term is proportional to $(\hat{Z}_1 + \hat{Z}_0)$ the third one is proportional to $(\hat{Z}_1 - \hat{Z}_0)$. Let us note that for $\vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(0)}$ one has

$$\begin{aligned}(\vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(0)}) |11\rangle &= |11\rangle, & (\vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(0)}) |\psi^+\rangle &= |\psi^+\rangle, \\ (\vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(0)}) |00\rangle &= |00\rangle, & (\vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(0)}) |\psi^-\rangle &= -3|\psi^-\rangle,\end{aligned}$$

where

$$|\psi^+\rangle = \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle), \quad |\psi^-\rangle = \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle).$$

Moreover, for $\frac{1}{2} (\hat{Z}_1 + \hat{Z}_0) \equiv \frac{1}{2} (\hat{Z} \otimes \hat{I} + \hat{I} \otimes \hat{Z})$ one has

$$\begin{aligned}\frac{1}{2} (\hat{Z}_1 + \hat{Z}_0) |11\rangle &= -|11\rangle, & \frac{1}{2} (\hat{Z}_1 + \hat{Z}_0) |\psi^+\rangle &= 0, \\ \frac{1}{2} (\hat{Z}_1 + \hat{Z}_0) |00\rangle &= |00\rangle, & \frac{1}{2} (\hat{Z}_1 + \hat{Z}_0) |\psi^-\rangle &= 0.\end{aligned}$$

For $\frac{1}{2} (\hat{Z}_1 - \hat{Z}_0) \equiv \frac{1}{2} (\hat{Z} \otimes \hat{I} - \hat{I} \otimes \hat{Z})$ one has

$$\begin{aligned}\frac{1}{2} (\hat{Z}_1 - \hat{Z}_0) |11\rangle &= 0, & \frac{1}{2} (\hat{Z}_1 - \hat{Z}_0) |\psi^+\rangle &= |\psi^-\rangle, \\ \frac{1}{2} (\hat{Z}_1 - \hat{Z}_0) |00\rangle &= 0, & \frac{1}{2} (\hat{Z}_1 - \hat{Z}_0) |\psi^-\rangle &= |\psi^+\rangle.\end{aligned}$$

Taking into consideration the above relationships, we obtain in the orthonormal basis of eigenstates

$$\{|11\rangle, |00\rangle, |\psi^+\rangle, |\psi^-\rangle\}$$

the following matrix of the considered Hamiltonian

$$\mathcal{H} = \begin{bmatrix} \mathcal{J} - B_+ & 0 & 0 & 0 \\ 0 & \mathcal{J} + B_+ & 0 & 0 \\ 0 & 0 & \mathcal{J} & B_- \\ 0 & 0 & B_- & -3\mathcal{J} \end{bmatrix}, \quad (16)$$

The eigenvalues of the Hamiltonian (16) are

$$\begin{aligned}\lambda_1 &= \mathcal{J} - B_+, & \lambda_3 &= -\mathcal{J} + \sqrt{4\mathcal{J}^2 + B_-^2}, \\ \lambda_2 &= \mathcal{J} + B_+, & \lambda_4 &= -\mathcal{J} - \sqrt{4\mathcal{J}^2 + B_-^2}.\end{aligned}$$

In the basis of eigenstates $\{|\chi_1\rangle, |\chi_2\rangle, |\chi_3\rangle, |\chi_4\rangle\}$ the Hamiltonian assumes the form

$$\mathcal{H} = \begin{bmatrix} \mathcal{J} - B_+ & 0 & 0 & 0 \\ 0 & \mathcal{J} + B_+ & 0 & 0 \\ 0 & 0 & -\mathcal{J} + \sqrt{4\mathcal{J}^2 + B_-^2} & 0 \\ 0 & 0 & 0 & -\mathcal{J} - \sqrt{4\mathcal{J}^2 + B_-^2} \end{bmatrix},$$

where $|\chi_1\rangle = |11\rangle$, $|\chi_2\rangle = |00\rangle$, while $|\chi_3\rangle$ and $|\chi_4\rangle$ are appropriate linear combinations of states $|\psi^+\rangle$ and $|\psi^-\rangle$.

It is easy to check that \hat{C}_Z has an eigenvalue $\lambda = -1$ with an associated eigenvector $|11\rangle$ and a threefold degenerated eigenvalue $\lambda = 1$ with an associated eigenvector span $\{|00\rangle, |\psi^+\rangle, |\psi^-\rangle\}$. Hence, it follows that the eigenstates of the Hamiltonian \mathcal{H} are also the eigenstates of the \hat{C}_Z . This result is not surprising, since in the standard basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$

$$\mathcal{H} = \begin{bmatrix} \mathcal{J} + B_1 + B_0 & 0 & 0 & 0 \\ 0 & -\mathcal{J} + B_1 - B_0 & 2\mathcal{J} & 0 \\ 0 & 2\mathcal{J} & -\mathcal{J} - B_1 + B_0 & 0 \\ 0 & 0 & 0 & \mathcal{J} - B_1 - B_0 \end{bmatrix},$$

$$\hat{C}_Z = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix},$$

hence one readily obtains that the commutator of \mathcal{H} and \hat{C}_Z is equal to 0

$$[\mathcal{H}, \hat{C}_Z] = 0.$$

The eigenstates of the Hamiltonian \mathcal{H} are the eigenstates of \hat{C}_Z , with the associated eigenvalues, respectively, -1 , 1 , 1 and 1 . One has

$$\begin{aligned}\langle \chi_1 | e^{-i\mathcal{H}\tau} | \chi_1 \rangle &= e^{-i\tau(\mathcal{J} - B_+)}, & \langle \chi_1 | \hat{C}_Z | \chi_1 \rangle &= -1, \\ \langle \chi_2 | e^{-i\mathcal{H}\tau} | \chi_2 \rangle &= e^{-i\tau(\mathcal{J} + B_+)}, & \langle \chi_2 | \hat{C}_Z | \chi_2 \rangle &= 1, \\ \langle \chi_3 | e^{-i\mathcal{H}\tau} | \chi_3 \rangle &= e^{-i\tau(-\mathcal{J} + \sqrt{4\mathcal{J}^2 + B_-^2})}, & \langle \chi_3 | \hat{C}_Z | \chi_3 \rangle &= 1, \\ \langle \chi_4 | e^{-i\mathcal{H}\tau} | \chi_4 \rangle &= e^{-i\tau(-\mathcal{J} - \sqrt{4\mathcal{J}^2 + B_-^2})}, & \langle \chi_4 | \hat{C}_Z | \chi_4 \rangle &= 1,\end{aligned}$$

thus the realization of the gate \hat{C}_Z will be possible (up to the global phase factor) if one can find such values of \mathcal{J} , B_1 , B_0 and τ that

$$\begin{aligned}rCl \quad e^{-i\tau(\mathcal{J} - B_+)} &= e^{i\tau(\mathcal{J} + B_+)} = e^{i\tau(-\mathcal{J} + \sqrt{4\mathcal{J}^2 + B_-^2})} \\ &= e^{i\tau(-\mathcal{J} - \sqrt{4\mathcal{J}^2 + B_-^2})}.\end{aligned} \quad (17)$$

The relationship (17) implies

$$e^{i\tau\sqrt{4\mathcal{J}^2 + B_-^2}} = \pm 1, \quad e^{i\tau B_+} = \pm i, \quad (18a)$$

$$e^{-2i\tau\mathcal{J}} = e^{i\tau B_+} e^{-i\tau\sqrt{4\mathcal{J}^2 + B_-^2}}. \quad (18b)$$

Relationships ((18a)) are satisfied for

$$B_+ = 2\mathcal{J}, \quad B_- = 2\sqrt{3}\mathcal{J}, \quad \tau = \frac{\pi}{4\mathcal{J}}, \quad (19)$$

hence

$$B_1 = (1 + \sqrt{3})\mathcal{J}, \quad B_0 = (1 - \sqrt{3})\mathcal{J}. \quad (20)$$

The values of the fields B_0 and B_1 are different, despite the fact that no one of the qubits is a priori distinguished. However, there is no contradiction, changing B_0 with B_1 yields the same transformation. The same applies to the case when B_0 and B_1 are time dependent.

4.2. Time dependent Hamiltonian. The case of time independent Hamiltonian, i.e., B_0 and B_1 fields constant within the $[0, \tau]$ period corresponds to the rectangular pulses of these fields. Such pulses are not physically realizable, thus the question arises whether it is possible to choose pulses changing in time, starting and ending in zero, but without any abrupt, step like changes. It turns out that it is possible to find such pulses.

Generally, when B_0 and B_1 fields change with time, the Hamiltonian of the system evolves with time according to the equation

$$\begin{aligned} \mathcal{H}(t) &= \mathcal{J}\vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(0)} + B_1(t)\hat{Z}_1 + B_0(t)\hat{Z}_0 \\ &= \mathcal{J}(\hat{X} \otimes \hat{X} + \hat{Y} \otimes \hat{Y} + \hat{Z} \otimes \hat{Z}) + B_1(t)(\hat{Z} \otimes \hat{I}) \\ &\quad + B_0(t)(\hat{I} \otimes \hat{Z}). \end{aligned}$$

The Hamiltonian matrix in the standard basis reads

$$\mathcal{H}(t) = \begin{bmatrix} \mathcal{J} + B_1(t) + B_0(t) & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\mathcal{J} + B_1(t) - B_0(t) & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2\mathcal{J} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2\mathcal{J} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\mathcal{J} - B_1(t) + B_0(t) & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathcal{J} - B_1(t) - B_0(t) & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

The state of the system $|\psi(t)\rangle$ evolves according to the Schrödinger equation

$$i\frac{d}{dt}|\psi(t)\rangle = \mathcal{H}(t)|\psi(t)\rangle, \quad |\psi_0\rangle = |\psi(0)\rangle. \quad (21)$$

Writing explicitly the state $|\psi(t)\rangle$ as the sum of real and imaginary parts

$$|\psi(t)\rangle = \text{Re}|\psi(t)\rangle + i\text{Im}|\psi(t)\rangle$$

one can reduce (21) to a real differential equation

$$\frac{d}{dt} \begin{bmatrix} \text{Re}|\psi(t)\rangle \\ \text{Im}|\psi(t)\rangle \end{bmatrix} = \begin{bmatrix} 0 & \mathcal{H}(t) \\ -\mathcal{H}(t) & 0 \end{bmatrix} \begin{bmatrix} \text{Re}|\psi(t)\rangle \\ \text{Im}|\psi(t)\rangle \end{bmatrix},$$

which can be solved numerically. The equation is solved on the time compartment $[0, \tau]$. We look for such $B_0(t)$ and

$B_1(t)$ that the evolution (21) realizes, up to the global phase factor, the following map:

$$|00\rangle \mapsto |00\rangle, \quad |01\rangle \mapsto |01\rangle, \quad |10\rangle \mapsto |10\rangle, \quad |11\rangle \mapsto -|11\rangle.$$

In other words we look for such $B_0(t)$ and $B_1(t)$ that solving on the compartment $[0, \tau]$ matrix differential equation

$$\frac{d}{dt}U(t) = -i\mathcal{H}(t)U(t), \quad (22)$$

with initial condition

$$U(0) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

we obtain

$$U(\tau) = e^{i\phi} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}, \quad (23)$$

for some global phase ϕ . Let us note that owing to the fact the operation (22) is unitary, and that $U(0)$ is a unitary, the $U(t)$ matrix remains unitary in any time moment $t \in [0, \tau]$.

Using the Matlab code, we have looked for, by trial and fail method, magnetic pulses (only the z component has been considered, the x and y components have been set to 0) of the form

$$B_\xi(t) = \sum_{k=1}^N A_{\xi,k} \sin(k\omega_0 t), \quad \omega_0 = \frac{\pi}{\tau} = 4\mathcal{J}, \quad (24)$$

where $\xi \in \{0, 1\}$. It turns out that already for $N = 1$ one can find the pulses of the form (24) that realize the \hat{C}_Z gate. Moreover, there are many pulses of the form (24), for different values of N that realize the \hat{C}_Z gate. A few of them are given in the Subsec. 4.3. The plots of these pulses, along with the corresponding plots of the time evolution of the appropriate elements of matrix U from the Eq. (22) are depicted in Figs. 1–10.

The results collected in the Subsec. 4.3 require a commentary. Let us note that in some case a better accuracy could be wished (it applies in particular to the $N = 4$ case – the values of the imaginary parts of $u_{11}(\tau)$ and $u_{44}(\tau)$ differ somewhat from zero). From the simulations we have performed, it follows that the accuracy can be increased at the expense of larger magnitudes of the pulses. For the pulses collected in the Subsec. 4.3, the magnitudes do not exceed $10\mathcal{J}$ (\mathcal{J} is a coupling constant). One can obtain the values of $u_{ii}(\tau)$, $i \in \{1, 2, 3, 4\}$ closer to 1 and -1 , respectively, but then the magnitudes of the pulses can achieve values of about $30\mathcal{J}$.

The case of pulses with one harmonic component is of particular interest. (Fig. 3, p. 385). The B_0 and B_1 pulses differ only by magnitude, thus by an appropriate choice of μ_0 and μ_1 values of magnetic moments one can realize the considered transformation just with one pulse (i.e., the same pulse for two spins). This is an important fact, since when the spins are close to each other, it is difficult to apply to them different values of magnetic field.

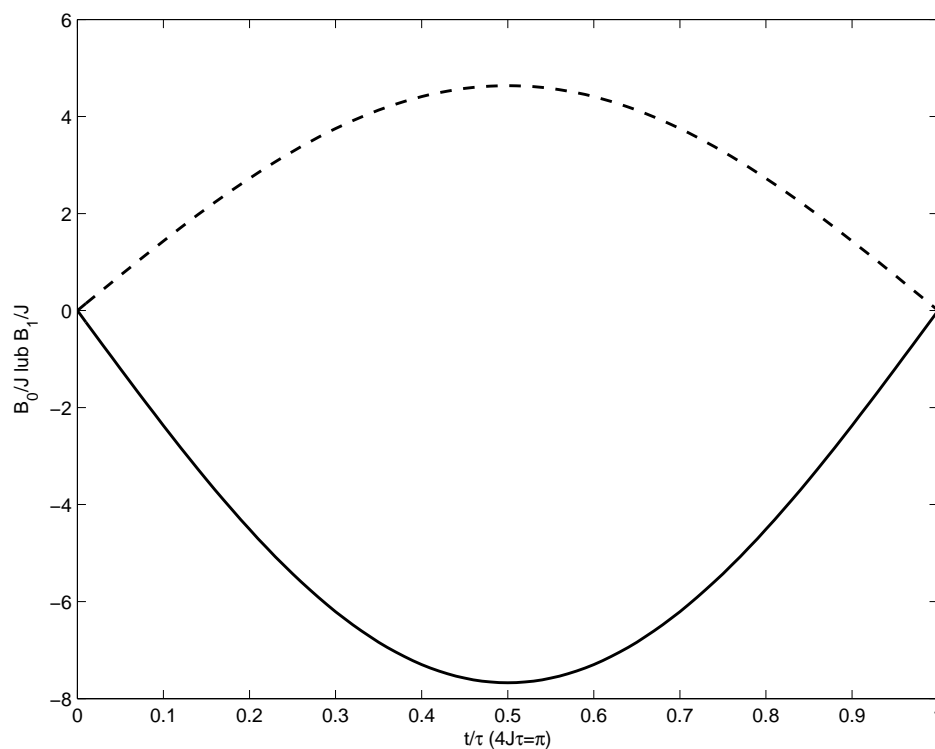


Fig. 1. Plots of magnetic pulses $B_\xi(t) = \sum_{k=1}^N A_{\xi,k} \sin k\omega_0 t$, $\xi \in \{0, 1\}$ for $N = 1$. Values of $A_{\xi,k}$ are given in Subsec. 4.3

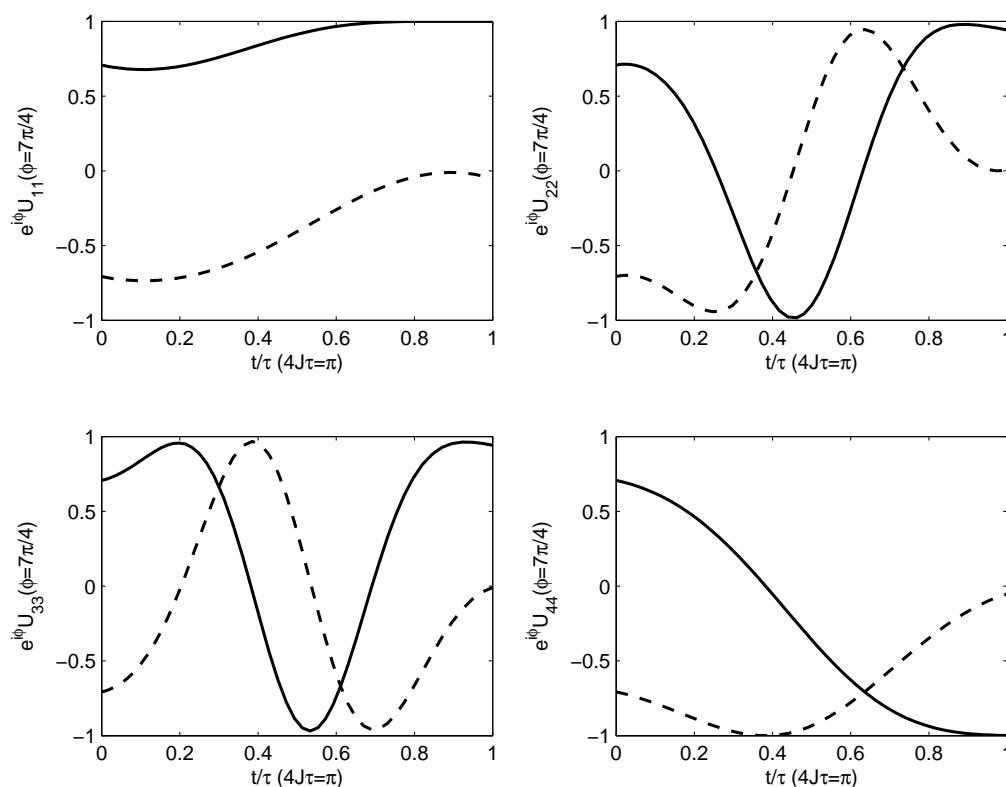


Fig. 2. Plots of the matrix elements of U in function of time for the unitary transformation realized by pulses $B_\xi(t) = \sum_{k=1}^N A_{\xi,k} \sin(k\omega_0 t)$, $\xi \in \{0, 1\}$ for $N = 1$. Continuous (dashed) lines correspond to real (imaginary) parts of the elements $u_{11}(t)$, $u_{22}(t)$, $u_{33}(t)$, $u_{44}(t)$, $t \in \{0, \tau\}$ of the matrix $e^{-i\phi} U(\tau)$ where $U(\tau)$ is given by formula (23)

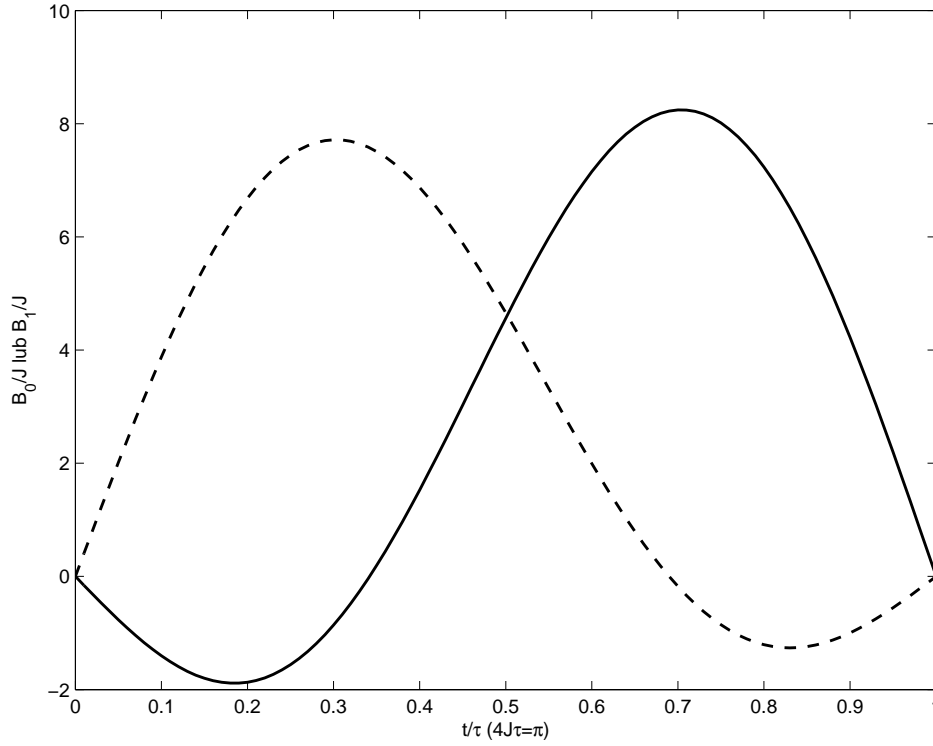


Fig. 3. Plots of magnetic pulses $B_\xi(t) = \sum_{k=1}^N A_{\xi,k} \sin k\omega_0 t$, $\xi \in \{0, 1\}$ for $N = 2$. Values of $A_{\xi,k}$ are given in Subsec. 4.3

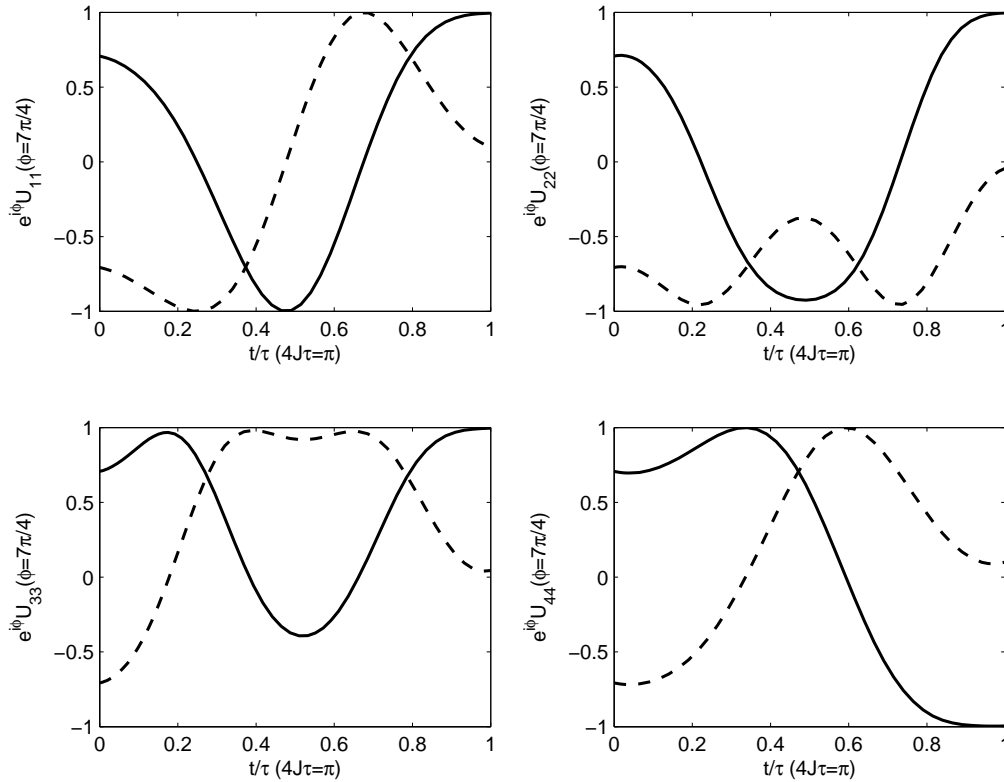


Fig. 4. Plots of the matrix elements of U in function of time for the unitary transformation realized by pulses $B_\xi(t) = \sum_{k=1}^N A_{\xi,k} \sin(k\omega_0 t)$, $\xi \in \{0, 1\}$ for $N = 2$. Continuous (dashed) lines correspond to real (imaginary) parts of the elements $u_{11}(t)$, $u_{22}(t)$, $u_{33}(t)$, $u_{44}(t)$, $t \in \{0, \tau\}$ of the matrix $e^{-i\phi} U(\tau)$ where $U(\tau)$ is given by formula (23)

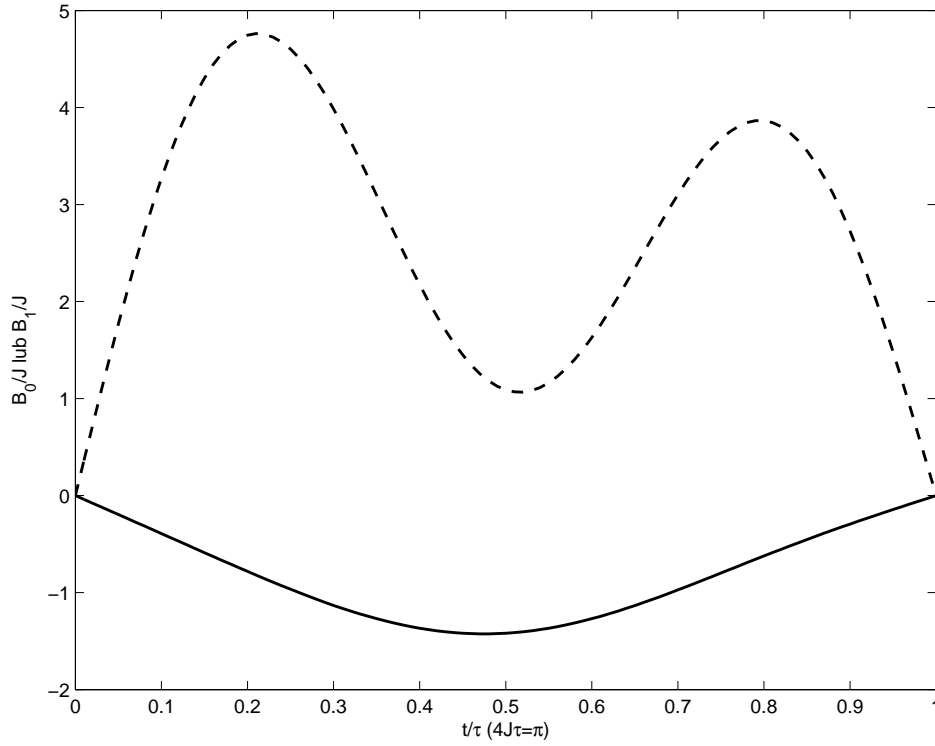


Fig. 5. Plots of magnetic pulses $B_\xi(t) = \sum_{k=1}^N A_{\xi,k} \sin k\omega_0 t$, $\xi \in \{0, 1\}$ for $N = 3$. Values of $A_{\xi,k}$ are given in Subsec. 4.3

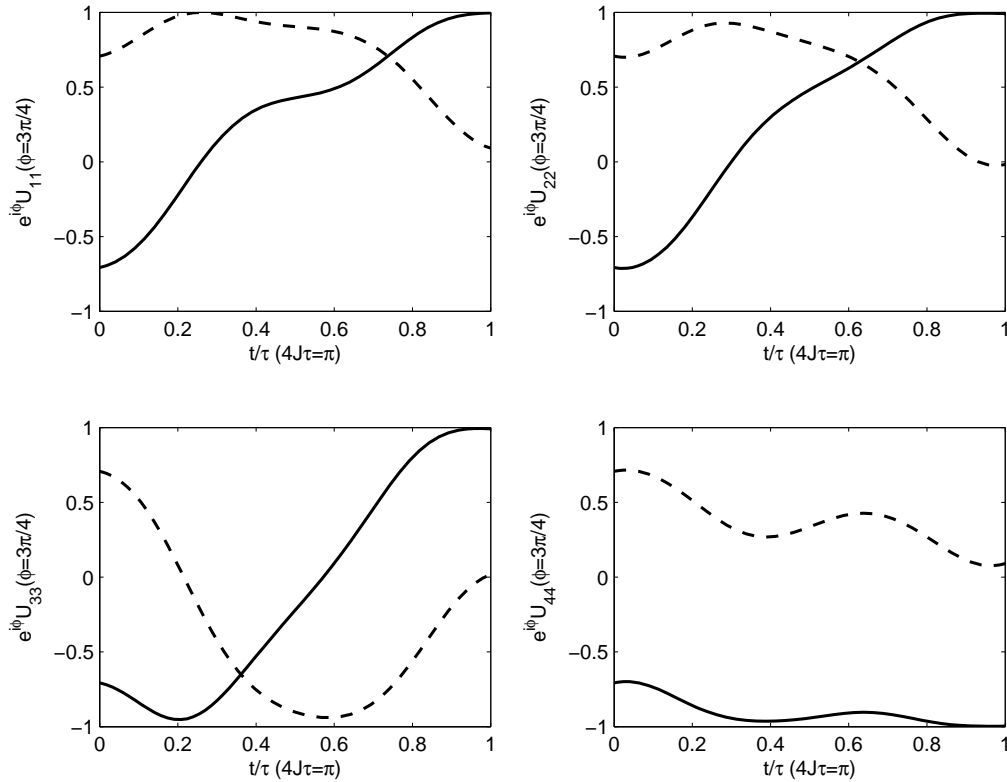


Fig. 6. Plots of the matrix elements of U in function of time for the unitary transformation realized by pulses $B_\xi(t) = \sum_{k=1}^N A_{\xi,k} \sin(k\omega_0 t)$, $\xi \in \{0, 1\}$ for $N = 3$. Continuous (dashed) lines correspond to real (imaginary) parts of the elements $u_{11}(t)$, $u_{22}(t)$, $u_{33}(t)$, $u_{44}(t)$, $t \in \{0, \tau\}$ of the matrix $e^{-i\phi} U(\tau)$ where $U(\tau)$ is given by formula (23)

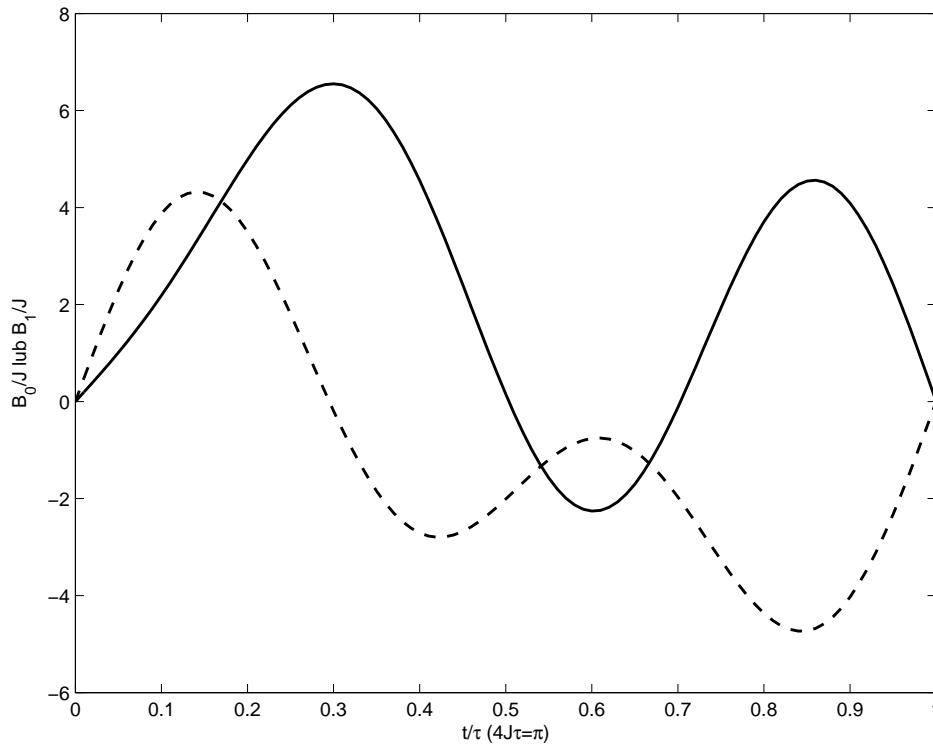


Fig. 7. Plots of magnetic pulses $B_\xi(t) = \sum_{k=1}^N A_{\xi,k} \sin k\omega_0 t$, $\xi \in \{0, 1\}$ for $N = 4$. Values of $A_{\xi,k}$ are given in Subsec. 4.3

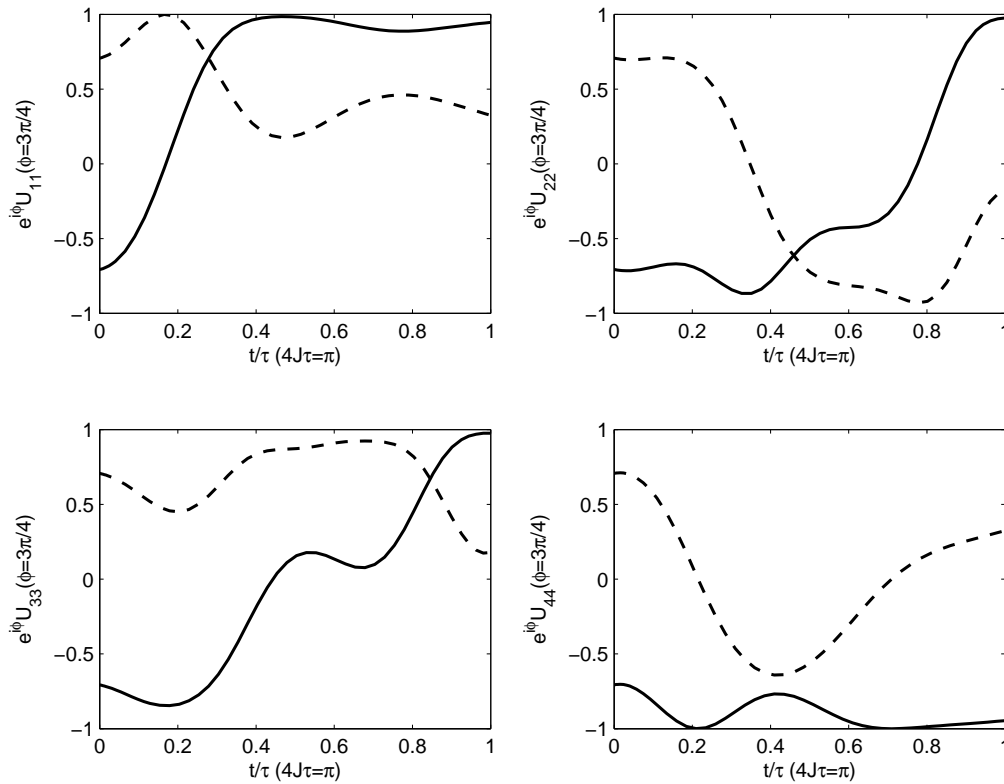


Fig. 8. Plots of the matrix elements of U in function of time for the unitary transformation realized by pulses $B_\xi(t) = \sum_{k=1}^N A_{\xi,k} \sin(k\omega_0 t)$, $\xi \in \{0, 1\}$ for $N = 4$. Continuous (dashed) lines correspond to real (imaginary) parts of the elements $u_{11}(t)$, $u_{22}(t)$, $u_{33}(t)$, $u_{44}(t)$, $t \in \{0, \tau\}$ of the matrix $e^{-i\phi} U(\tau)$ where $U(\tau)$ is given by formula (23)

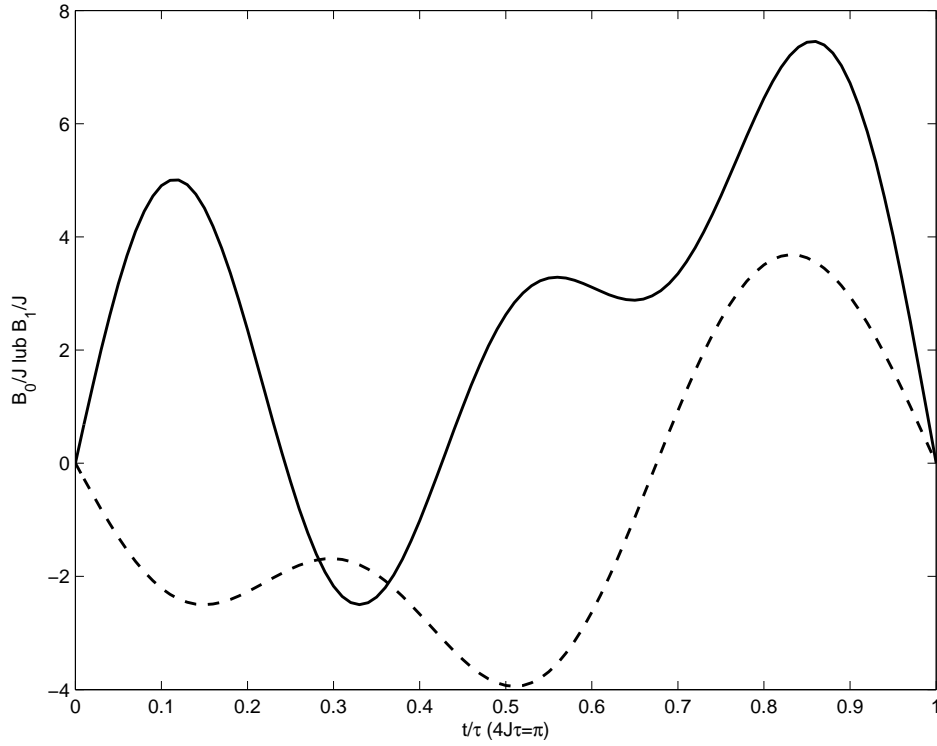


Fig. 9. Plots of magnetic pulses $B_\xi(t) = \sum_{k=1}^N A_{\xi,k} \sin k\omega_0 t$, $\xi \in \{0, 1\}$ for $N = 5$. Values of $A_{\xi,k}$ are given in Subsec. 4.3

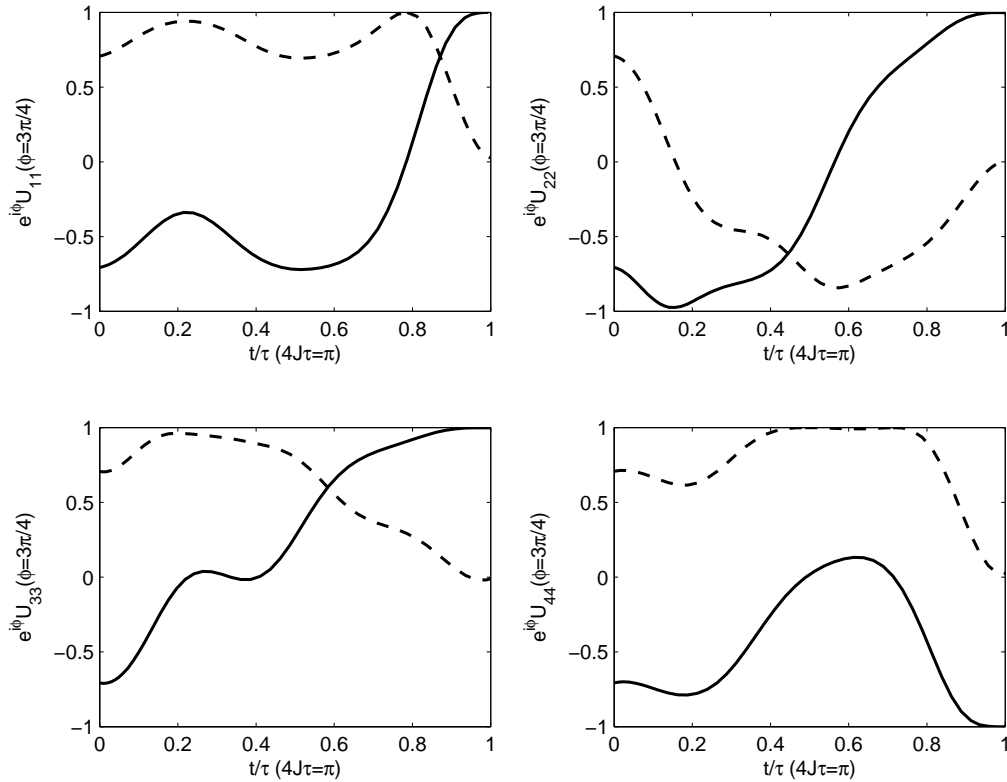


Fig. 10. Plots of the matrix elements of U in function of time for the unitary transformation realized by pulses $B_\xi(t) = \sum_{k=1}^N A_{\xi,k} \sin(k\omega_0 t)$, $\xi \in \{0, 1\}$ for $N = 5$. Continuous (dashed) lines correspond to real (imaginary) parts of the elements $u_{11}(t)$, $u_{22}(t)$, $u_{33}(t)$, $u_{44}(t)$, $t \in \{0, \tau\}$ of the matrix $e^{-i\phi}U(\tau)$ where $U(\tau)$ is given by formula (23)

One should also pay an attention to the phase ϕ appearing in the formula (23). It turns out that for all pulses presented in Subsec. 4.3, it is equal $3\pi/4$ or $7\pi/4$. However, explanation of this fact remains an open problem.

4.3. Simulation results. This section contains the specific magnetic pulses realizing the \hat{C}_Z gate. All pulses are of the form $B_\xi(t) = \sum_{k=1}^N A_{\xi,k} \sin k\omega_0 t$, where $\xi \in \{0, 1\}$, and $N \in \{1, 2, 3, 4, 5\}$, $\omega_0 = 4\mathcal{J}$. There were also provided the values $u_{11}(\tau) = e^{-i\phi}U_{11}(\tau)$, $u_{22}(\tau) = e^{-i\phi}U_{22}(\tau)$, $u_{33}(\tau) = e^{-i\phi}U_{33}(\tau)$, $u_{44}(\tau) = e^{-i\phi}U_{44}(\tau)$, where $U_{11}(\tau)$, $U_{22}(\tau)$, $U_{33}(\tau)$, $U_{44}(\tau)$ are the elements of the unitary matrix $U(\tau)$ from the relationship (23), and $\tau = \frac{\pi}{4\mathcal{J}}$. The desired values are, respectively, $u_{11}(\tau) = u_{22}(\tau) = u_{33}(\tau) = 1$, $u_{44}(\tau) = -1$.

1. $N = 1$

$A_{0,1} = -7.6733$	$A_{1,1} = 4.6370$
$u_{1,1}(\tau) = 0.9986 - 0.0526i$	
$u_{2,2}(\tau) = 0.9416 + 0.0094i$	
$u_{3,3}(\tau) = 0.9416 - 0.0090i$	
$u_{4,4}(\tau) = -0.9986 - 0.0526i$	

2. $N = 2$

$A_{0,1} = 4.5631$	$A_{1,1} = 4.6601$
$A_{0,2} = -4.7861$	$A_{1,2} = 4.1489$
$u_{1,1}(\tau) = 0.9950 + 0.1003i$	
$u_{2,2}(\tau) = 0.9963 - 0.0440i$	
$u_{3,3}(\tau) = 0.9962 + 0.0442i$	
$u_{4,4}(\tau) = -0.9949 + 0.1005i$	

3. $N = 3$

$A_{0,1} = -1.3334$	$A_{1,1} = 3.4707$
$A_{0,2} = -0.0837$	$A_{1,2} = 0.4637$
$A_{0,3} = 0.0857$	$A_{1,3} = 2.3813$
$u_{1,1}(\tau) = 0.9959 + 0.0908i$	
$u_{2,2}(\tau) = 0.9915 - 0.0178i$	
$u_{3,3}(\tau) = 0.9915 + 0.0178i$	
$u_{4,4}(\tau) = -0.9959 + 0.0909i$	

4. $N = 4$

$A_{0,1} = 2.9188$	$A_{1,1} = -1.5230$
$A_{0,2} = 2.0895$	$A_{1,2} = 2.5355$
$A_{0,3} = 2.7661$	$A_{1,3} = 0.4873$
$A_{0,4} = -2.2924$	$A_{1,4} = 2.5910$
$u_{1,1}(\tau) = 0.9460 + 0.3246i$	
$u_{2,2}(\tau) = 0.9757 - 0.1785i$	
$u_{3,3}(\tau) = 0.9755 + 0.1786i$	
$u_{4,4}(\tau) = -0.9459 + 0.3246i$	

5. $N = 5$

$A_{0,1} = 2.8670$	$A_{1,1} = -1.7253$
$A_{0,2} = -2.5268$	$A_{1,2} = -2.2067$
$A_{0,3} = 2.8575$	$A_{1,3} = 1.7149$
$A_{0,4} = 0.6084$	$A_{1,4} = -1.3457$
$A_{0,5} = 2.6145$	$A_{1,5} = -0.4872$
$u_{1,1}(\tau) = 1.0003 + 0.0249i$	
$u_{2,2}(\tau) = 0.9976 + 0.0107i$	
$u_{3,3}(\tau) = 0.9976 - 0.0107i$	
$u_{4,4}(\tau) = -1.0001 + 0.0251i$	

5. Conclusions

The problem of the CNOT gate (realized as a system of two interacting spins) control has been addressed in the paper, in particular, the control of CNOT gate via magnetic pulses has been analyzed. It was shown that there exist such pulses that realize the CNOT gate, and that they can be numerically computed by a simple trial and the failure method.

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