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Feasibility of the controlled-NOT gate from certain model Hamiltonians

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Abstract

The controlled-NOT (CNOT) gate is widely used in quantum circuits and in current and proposed quantum computing technologies. We investigate the feasibility and minimal implementation of CNOT from specific model Hamiltonian operators that have appeared in the literature. We follow an algebraic approach that provides an analytic solution. Our results are relevant to effective two-qubit Hamiltonians currently being considered for spin-based, superconductivity-based and other implementations of quantum computing.

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Introduction

There has been much interest of late in characterizing two-qubit operations, optimizing the number of quantum logic gates in small circuits and developing minimal universal bases of quantum gates [1–9]. In order to have a universal basis of quantum gates [10], it is necessary to have a two-qubit operator that at least partially entangles two-qubit states. Two common entanglers are the controlled-NOT (CNOT) and SWAP$^\alpha$ gates, with $0 < \alpha < 1$.

In this paper, we supplement existing work on the feasibility and minimal implementation of two-qubit operations in terms of the widely used CNOT gate. One motivation for this is determining the practicality of CNOT and two-qubit gates derived from it for optically based type II (or hybrid) quantum computing. More immediate, some recent investigation developed a combination of analytic and numerical tests for CNOT feasibility [1, 11], and some questions corresponding to certain Hamiltonian operators were left open. We address these topics, providing a fully analytic solution, and additionally present some extensions.

We are concerned with whether certain parameterized Hamiltonians can generate a CNOT up to local (single-qubit) gates in a certain time. An initial question is whether this is possible at all. If so, we then seek an analytic result for the time to evolve to the CNOT gate, t_{CNOT}.

As mentioned, a reason for investigating the feasibility and minimal implementation of specified two-qubit operations is provided by type II quantum computing [12–14]. Within this approach, a small number of qubits per node of a regular lattice is used. In addition to (re)initialization, the steps for running a quantum lattice gas algorithm on such an architecture are collision, qubit state read out and streaming. In the streaming step, the qubit states are communicated to the nearest neighbours of the lattice, while the collision operation is quantum in nature. The unitary collision operator will presumably be more efficiently implemented in terms of one entangler than another. To date, quantum lattice gas algorithms have been simulated with only two or three qubits per node, although this is by no means necessary. The collision operator for the most part has been based upon the $\mathrm{SWAP}^{1/2}$ gate. Besides current NMR implementation [15], superconducting qubits [16–20] and optical qubits appear promising.

Various authors have numerically sought gate implementations, even for two or three qubits. A certain characteristic polynomial derived from the evolution operator at uniformly spaced points in time has been evaluated in [1, 11]. We show that this can be avoided in finding t_{CNOT}. In contrast, references such as [19, 20] numerically seek an overall quantum gate that implements a given unitary transformation, instead of using a sequence of elementary gates. This is done by working in the control-parameter space of time-dependent coefficients of the Hamiltonian. In addition, optimal implementation of two-qubit controlled-unitary operations has been studied in [21]. It provides a compendium of numerical tests that detect when zero, one or two CNOT gates are required.

In the next section, we first recall some background, note some properties of unitary operators that we use and give some examples. We then address some specific Hamiltonians H and the feasibility of obtaining the CNOT gate. After this we discuss alternative operator methods for obtaining the matrix exponentials of interest for the quantum evolution operator. While we concentrate on Hamiltonians of special eigenstructure, we briefly mention some general techniques. We then provide a number of extensions, including to Hamiltonians with time-dependent coefficients, and finish with a brief summary.

It may be worth pointing out that Hamiltonians commonly occurring in quantum computing have special structure, implying additional properties beyond mere Hermiticity. In addition, the Hamiltonians of interest for quantum computing are those that may be efficiently simulated, i.e., simulated with a number of logic gates that is polynomial instead of exponential in the number of qubits.

Notation and method

We adopt the notation and conventions of [1, 3]. As usual, $U(N)$ denotes the group of $N \times N$ unitary matrices and $SU(N)$ the group of such matrices with determinant 1 with $N^2 - 1$ parameters. For $u \in U(4)$ we put $\gamma(u) = u\sigma_y^{\otimes 2}u^T\sigma_y^{\otimes 2}$. Here σ_j are the standard Pauli matrices and T denotes transposition. For a gate $g \in U(n)$ we put $\chi(g) = \det(xI_n - g)$ for the characteristic polynomial, where I_n is the $n \times n$ identity matrix. For $n = 4$, we require $g \in SU(4)$, so that the global phase of two-qubit unitaries is fixed to within factors of ± 1 or $\pm\mathrm{i}$. We note the properties $\gamma(cu) = c^2\gamma(u)$, $\gamma(I_4) = I_4$ and $\gamma(\mathrm{e}^{\pm\mathrm{i}\pi/4}\ \mathrm{CNOT}) = \mp\mathrm{i}\sigma_z \otimes \sigma_x$ for c a constant and $\mathrm{CNOT} = \frac{1}{2}(I_2 + \sigma_z) \otimes I_2 + \frac{1}{2}(I_2 - \sigma_z) \otimes \sigma_x$. Here $\det(\mathrm{CNOT}) = -1$ and we normalize the corresponding gate to be in $SU(4)$ with the factor $\mathrm{e}^{\pm\mathrm{i}\pi/4}$.

In particular, for u and v in $SU(4)$, they are equivalent up to local gates if and only if $\chi[\gamma(u)] = \chi[\pm\gamma(v)]$ [1]. An operator $u \in SU(4)$ can be simulated with precisely one CNOT gate if and only if $\chi[\gamma(u)] = (x^2 + 1)^2$ [1] (proposition 3).

We note the following scaling property of the characteristic polynomial that is especially pertinent in the case that an operator in $SU(4)$ is implementable in terms of two CNOTs and local gates [1] (proposition 4). If the characteristic polynomial has coefficients g_j, $\chi(g) = P(x) = x^4 + g_3x^3 + g_2x^2 + g_1x + g_0$, then for a constant c with $|c| = 1$, $\chi(cg) =$

$x^4+cg_3x^3+c^2g_2x^2+c^3g_1x+c^4g_0$. In particular, if $P(x)=x^4+g_2x^2+g_0$ for g, then cg has the characteristic polynomial $x^4+g_2c^2x^2+c^4g_0$. So if g_2 and g_0 are real coefficients, g_2c^2 and c^4g_0 remain real if $c=\pm 1$ or $\pm\mathrm{i}$. Of course, if $g \in SU(4)$, then necessarily $g_0 = 1 = \det(g) \equiv |g|$ and g_2 is real.

For consistency with [1, 11] we take in what follows $U(t) = \exp(\mathrm{i}Ht)$ for the evolution operator, where $\hbar = 1$ for convenience, whereas it is probably more conventional to take $U(t) = \exp(-\mathrm{i}Ht)$ as the solution of the time-dependent Schrödinger equation $\mathrm{i}\hbar\dot{U} = HU(t)$ with initial condition $U(0) = I$, the identity operator. These conventions should be kept in mind in regards to physical implementations.

As a first example, consider the two-qubit gate

$$\mathrm{SWAP}^{\alpha} = \frac{1}{2}\begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 1+\mathrm{e}^{\mathrm{i}\alpha\pi} & 1-\mathrm{e}^{\mathrm{i}\alpha\pi} & 0 \\ 0 & 1-\mathrm{e}^{\mathrm{i}\alpha\pi} & 1+\mathrm{e}^{\mathrm{i}\alpha\pi} & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix}. \tag{1}$$

It is known that, when measured in terms of the number of gates, SWAP^{α} and CNOT gates are equally efficient in realizing any two-qubit quantum operation. Furthermore, arbitrary two-qubit unitary operations require only three SWAP^{α} gates with certain values of α and six single-qubit gates [2].

We have $|\mathrm{SWAP}^{\alpha}| = \mathrm{e}^{\mathrm{i}\alpha\pi}$ and find that

$$\gamma\left(\frac{\mathrm{SWAP}^{\alpha}}{|\mathrm{SWAP}^{\alpha}|^{1/4}}\right) = \mathrm{e}^{-\mathrm{i}\alpha\pi/2}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \mathrm{e}^{\mathrm{i}\alpha\pi}\cos\alpha\pi & -\mathrm{i}\,\mathrm{e}^{\mathrm{i}\alpha\pi}\sin\alpha\pi & 0 \\ 0 & -\mathrm{i}\,\mathrm{e}^{\mathrm{i}\alpha\pi}\sin\alpha\pi & \mathrm{e}^{\mathrm{i}\alpha\pi}\cos\alpha\pi & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \tag{2}$$

and

$$\chi\left[\gamma\left(\frac{\mathrm{SWAP}^{\alpha}}{|\mathrm{SWAP}^{\alpha}|^{1/4}}\right)\right] = x^4 - \mathrm{e}^{-\mathrm{i}\alpha\pi/2}(\mathrm{e}^{2\mathrm{i}\alpha\pi}+3)x^3 + 3\,\mathrm{e}^{-\mathrm{i}\alpha\pi}(\mathrm{e}^{2\mathrm{i}\alpha\pi}+1)x^2 - \mathrm{e}^{-3\mathrm{i}\alpha\pi/2}(1+3\,\mathrm{e}^{2\mathrm{i}\alpha\pi})x + 1. \tag{3}$$

Then $\mathrm{Tr}\big[\gamma\big(\frac{\mathrm{SWAP}^{\alpha}}{|\mathrm{SWAP}^{\alpha}|^{1/4}}\big)\big] = 2(\mathrm{e}^{-\mathrm{i}\alpha\pi/2} + \mathrm{e}^{\mathrm{i}\alpha\pi/2}\cos\alpha\pi)$ has vanishing imaginary part only when α is an even integer. Since $\alpha = 0$ is the trivial case of the identity matrix from SWAP^{α}, it generally requires three CNOT gates and single-qubit gates to simulate SWAP^{α} [1]. For $\alpha = 1$ we recover the well-known result that SWAP is equivalent to three CNOT gates. Despite the known result that one CNOT can be realized by two $\mathrm{SWAP}^{1/2}$ gates and single-qubit gates [2], a reciprocal result for $\mathrm{SWAP}^{1/2}$ from two CNOT and single-qubit gates does not seem to hold.

Timing a Hamiltonian to produce CNOT

Consider the two-qubit Hamiltonian

$$H_w \equiv wI_2 \otimes \sigma_z + \sigma_x \otimes \sigma_x, \tag{4}$$

where $-1 \leqslant w \leqslant 1$. In this section, we show, among other results, that H_w generates a CNOT gate and that the time for which this occurs is

$$t_{\mathrm{CNOT}} = \frac{1}{2}\frac{\cos^{-1}(-w^2)}{\sqrt{1+w^2}}. \tag{5}$$

This formula subsumes a numerical result restricted to the special value of $w = 0.42$ [1, 11].

We first note the special structure of

$$H_{bw} \equiv wI_2 \otimes \sigma_z + b\sigma_x \otimes \sigma_x = H_{bw}^{(1)} + H_{bw}^{(2)} \equiv \begin{bmatrix} w & 0 & 0 & b \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ b & 0 & 0 & -w \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & -w & b & 0 \\ 0 & b & w & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \tag{6}$$

where b is a real number. While in general $\exp(A + B) \neq \exp(A)\exp(B)$ for operators A and B, here we have $\exp(\mathrm{i}H_{bw}t) = \exp\big(\mathrm{i}H_{bw}^{(1)}t\big)\exp\big(\mathrm{i}H_{bw}^{(2)}t\big)$. Not only do $H_{bw}^{(1)}$ and $H_{bw}^{(2)}$ commute, the separate products $H_{bw}^{(1)}H_{bw}^{(2)} = H_{bw}^{(2)}H_{bw}^{(1)} = 0$. This reflects the fact that $H_{bw}^{(1)}$ and $H_{bw}^{(2)}$ act on distinct subspaces of $C^2 \otimes C^2$. The eigenvalues of H_{bw} are simply $\pm\sqrt{w^2 + b^2}$, each of multiplicity two, and $\exp(\mathrm{i}H_{bw}t)$ has the same main-diagonal-plus-cross-diagonal form as H_{bw} itself.

Therefore, it suffices to determine the evolution operator $U_{bw}(t) = \exp(\mathrm{i}H_{bw}t)$ simply from the known result for the matrix exponential of a 2×2 matrix. We have, putting $f \equiv \sqrt{(a-d)^2 + 4bc}$,

$$\exp\left(\begin{bmatrix} a & b \\ c & d \end{bmatrix}\right) = \frac{1}{f}$$
$$\times \begin{bmatrix} \mathrm{e}^{(a+d)/2}[f\cosh(f/2) + (a-d)\sinh(f/2)] & 2b\,\mathrm{e}^{(a+b)/2}\sinh(f/2) \\ 2c\,\mathrm{e}^{(a+b)/2}\sinh(f/2) & \mathrm{e}^{(a+d)/2}[f\cosh(f/2) + (d-a)\sinh(f/2)] \end{bmatrix}. \tag{7}$$

We may note the simplification that occurs in this equation for $a = -d$, and that this is precisely the case for $H_{bw}^{(j)}$ in equation (6). In this instance, the matrix $\left[\begin{smallmatrix} a & b \\ c & -a \end{smallmatrix}\right]$ has eigenvalues of opposite sign, $\pm f/2$.

Putting $x \equiv \sqrt{w^2 + b^2}$ and noting $\cosh(\mathrm{i}t) = \cos t$, $\sinh(\mathrm{i}t) = \mathrm{i}\sin t$, we obtain the symmetric unitary matrix

$$xU_{bw}(t) = x\cos(xt)I_4 + \mathrm{i}\sin(xt)[wI_2 \otimes \sigma_z + b\sigma_x \otimes \sigma_x]. \tag{8}$$

Without loss of generality, we may take $b = 1$, that amounts only to a scaling of the Hamiltonian H_{bw} with $w \to w/b$. As $U_{bw}(t)$ is a symmetric unitary, its determinant may only take the values ± 1. Indeed, as H_{bw} is traceless, $|U_{bw}(t)| = 1$. We find that, with $U_w(t) \equiv \exp(\mathrm{i}H_w t)$,

$$x^2\gamma(U_w) = [w^2 + \cos(2xt)]I_4 + \mathrm{i}w[-1 + \cos(2xt)]\sigma_x \otimes \sigma_y + \mathrm{i}x\sin(2xt)\sigma_x \otimes \sigma_x. \tag{9}$$

We then ask when $\chi[\gamma(U_w(t))] = (x^2 + 1)^2$. This gives the condition

$$\frac{4}{x^2}[w^2 + \cos(2xt)] = 0, \tag{10}$$

whence equation (5) follows. At the time $t = t_{\mathrm{CNOT}}$ we have, with $w' \equiv \sqrt{1 - w^2}$,

$$U_w(t) = \frac{1}{\sqrt{2}}(w'I_4 + \mathrm{i}wI_2 \otimes \sigma_z + \mathrm{i}\sigma_x \otimes \sigma_x)$$
$$= \frac{1}{\sqrt{2}}\begin{bmatrix} \mathrm{i}w + w' & 0 & 0 & \mathrm{i} \\ 0 & -\mathrm{i}w + w' & \mathrm{i} & 0 \\ 0 & \mathrm{i} & \mathrm{i}w + w' & 0 \\ \mathrm{i} & 0 & 0 & -\mathrm{i}w + w' \end{bmatrix}. \tag{11}$$

We note that a condition similar to equation (10) arose [22] (p 11) in connection with generating a CNOT gate from the Hamiltonian

$$H_{yy} = g_{1x}\sigma_x^1 + g_{1z}\sigma_z^1 + g_{2x}\sigma_x^2 + g_{2z}\sigma_z^2 + J\sigma_y^1\sigma_y^2. \tag{12}$$

In fact, given $f_1 + f_2 = 2\sqrt{g_{1x}^2 + g_{1z}^2}$ and $f_1 - f_2 = 2\sqrt{g_{2x}^2 + g_{2z}^2}$, and taking $J = 1$, the required time satisfies

$$t = \frac{\cos^{-1}\left(-f_j^2\right) + 2\pi n_j}{2\sqrt{f_j^2 + 1}}, \qquad j = 1, 2, \tag{13}$$

where n_j are integers and the principal branch is taken for the arccosine function. The minimal time solution numerically determined together with f_1 and f_2 in [22] corresponds to $n_1 = n_2 = 1$.

A semianalytic solution of equation (13) is possible, requiring only root finding to determine f_1. The right-hand side of that equation for $n_1 = 1$ will have a minimum near $f_1 \approx 0.95$, with the precise value determined by the condition of zero derivative with $f_1 \neq 0$:

$$\cos^{-1}\left(-f_1^2\right) + 2\pi = 2\sqrt{\frac{1 + f_1^2}{1 - f_1^2}}, \qquad 0 < f_1 < 1. \tag{14}$$

Substitution of this expression into equation (13) at $n_1 = n_2 = 1$ gives the remarkably compact result

$$t_{\text{CNOT}} = \frac{1}{\sqrt{1 - f_1^2}}. \tag{15}$$

Therefore we obtain the values $f_1 = f_2 \simeq 0.951\,640\,216\,44$ and $t_{\text{CNOT}} \simeq 3.255\,052\,116\,05$.

Now consider the isotropic Heisenberg (exchange) Hamiltonian

$$H_{XYZ} = \sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y + \sigma_z \otimes \sigma_z. \tag{16}$$

We have $|\mathrm{e}^{\mathrm{i}H_{XYZ}t}| = 1$ and find that

$$\gamma(\mathrm{e}^{\mathrm{i}H_{XYZ}t}) = \begin{bmatrix} \mathrm{e}^{2\mathrm{i}t} & 0 & 0 & 0 \\ 0 & \cos 4t(\cos 2t - \mathrm{i}\sin 2t) & \mathrm{i}\,\mathrm{e}^{-2\mathrm{i}t}\sin 4t & 0 \\ 0 & \mathrm{i}\,\mathrm{e}^{-2\mathrm{i}t}\sin 4t & \cos 4t(\cos 2t - \mathrm{i}\sin 2t) & 0 \\ 0 & 0 & 0 & \mathrm{e}^{2\mathrm{i}t} \end{bmatrix}, \tag{17}$$

and

$$\chi[\gamma(\mathrm{e}^{\mathrm{i}H_{XYZ}t})] = (x - \mathrm{e}^{2\mathrm{i}t})^3(x - \mathrm{e}^{-6\mathrm{i}t}). \tag{18}$$

Then it is possible to find times t such that this characteristic polynomial assumes the form of $(x \pm 1)^4$. However, due to the asymmetry in the two x-dependent factors on the right-hand side of equation (18), it is not possible for $\chi[\gamma(\mathrm{e}^{\mathrm{i}H_{XYZ}t})]$ to take the form of $(x^2 + 1)^2$. So it is possible according to the value of t for $\exp(\mathrm{i}H_{XYZ}t)$ to be either in the equivalence class with no CNOT or two CNOT gates, but not a single CNOT. This proves that H_{XYZ} cannot be timed to generate CNOT. This nonfeasibility question was left open in [1]. However, it was just previously resolved in [7] (section VA), where it was shown that H_{XYZ} may implement $\text{SWAP}^{1/2}$ and its inverse and no other perfect entanglers. We have given an alternative demonstration.

Alternative techniques for the matrix exponential

Based upon tensor product properties, there are many different ways in which to find the quantum evolution operator from the Hamiltonians of interest in this paper. We illustrate several of these in this section. These techniques likely have other applications, as many generalizations are possible.

As a first simple example, consider the Hamiltonian H_{bw} of equation (6). We find that $H_{bw}^2 = (w^2+b^2)I_4$. By forming the Maclaurin series for $U_{bw}(t) = \exp(\mathrm{i}H_{bw}t)$ we then obtain

$$U_{bw}(t) = \cos(xt)I_4 + \frac{\mathrm{i}}{x}\sin(xt)H_{bw}. \tag{19}$$

We thus recover equation (8).

We next present various methods for deriving the evolution operator and other properties following from the Hamiltonian H_{XYZ} of equation (16). Again based upon the properties of tensor products of Pauli matrices, we find the relation

$$H_{XYZ}^2 = 3I_4 - 2H_{XYZ}. \tag{20}$$

This property suffices to find all nonnegative integers powers of H_{XYZ} and indeed then all analytic functions of it. If we put $H_{XYZ}^j = a_j H_{XYZ} + b_j I_4$, with a_j and b_j integer coefficients to be determined, we have by equation (20) that

$$H_{XYZ}^{j+1} = 3a_j I_4 + (b_j - 2a_j)H_{XYZ}. \tag{21}$$

Therefore, we find the recursion relations

$$b_{j+1} = 3a_j, \qquad a_{j+1} = b_j - 2a_j, \tag{22}$$

with the initial values $a_1 = 1$ and $b_1 = 0$. The solution of equation (22),

$$a_j = \tfrac{1}{4}[1-(-3)^j], \qquad b_j = \tfrac{1}{4}[3+(-3)^j], \tag{23}$$

exhibits the relation $a_j + b_j = 1$, $j \geqslant 1$, that may otherwise be readily verified. Indeed, from equation (22) we have $b_{j+1} + a_{j+1} = b_j + a_j = a_1 + b_1 = 1$ and then the single equation for say b_j is $b_{j+1} = 3 - 3b_j$. We have found

$$H_{XYZ}^j = \tfrac{1}{4}\{[1-(-3)^j]H_{XYZ} + [3+(-3)^j]I_4\}, \tag{24}$$

and this in turn yields

$$U_{XYZ}(t) \equiv \mathrm{e}^{\mathrm{i}H_{XYZ}t} = \tfrac{1}{4}[2\mathrm{i}\,\mathrm{e}^{-\mathrm{i}t}\sin 2t\,H_{XYZ} + (\mathrm{e}^{-3\mathrm{i}t} + 3\,\mathrm{e}^{\mathrm{i}t})I_4]. \tag{25}$$

We may note in passing that each tensor product term in H_{XYZ} commutes with the others. Therefore, we have

$$\begin{aligned} U_{XYZ}(t) &= \exp(\mathrm{i}\sigma_x\otimes\sigma_x t)\exp(\mathrm{i}\sigma_y\otimes\sigma_y t)\exp(\mathrm{i}\sigma_z\otimes\sigma_z t) \\ &= (\cos t I_2 + \mathrm{i}\sin t\sigma_x\otimes\sigma_x)(\cos t I_2 + \mathrm{i}\sin t\sigma_y\otimes\sigma_y)(\cos t I_2 + \mathrm{i}\sin t\sigma_z\otimes\sigma_z). \end{aligned} \tag{26}$$

Again using properties such as $(\sigma_x\otimes\sigma_x)(\sigma_y\otimes\sigma_y)(\sigma_z\otimes\sigma_z) = -I_4$ we obtain the alternative expression

$$U_{XYZ}(t) = (\cos^3 t + \mathrm{i}\sin^3 t)I_4 + \mathrm{i}\,\mathrm{e}^{\mathrm{i}t}\cos t\sin t\,H_{XYZ}. \tag{27}$$

Finally, as a third method for dealing with H_{XYZ}, we may apply the operator Schmidt decomposition of the SWAP gate,

$$\mathrm{SWAP} = \tfrac{1}{2}(I_2\otimes I_2 + \sigma_x\otimes\sigma_x + \sigma_y\otimes\sigma_y + \sigma_z\otimes\sigma_z). \tag{28}$$

This gives $H_s \equiv H_{XYZ}/2 = \mathrm{SWAP} - I_4/2$ and is again very convenient for exponentiating H_{XYZ} as of course SWAP commutes with the identity operator. We have $\exp(\mathrm{i}H_s t) =$

$\exp(\mathrm{iSWAP}t)\exp(-\mathrm{i}I_4 t/2)$, where the latter factor is the diagonal matrix $\exp(-\mathrm{i}I_4 t/2) = \mathrm{diag}(\mathrm{e}^{-\mathrm{i}t/2}, \mathrm{e}^{-\mathrm{i}t/2}, \mathrm{e}^{-\mathrm{i}t/2}, \mathrm{e}^{-\mathrm{i}t/2})$. Since $\mathrm{SWAP}^2 = I_4$, we have

$$\mathrm{e}^{\mathrm{iSWAP}t} = \cos t\, I_4 + \mathrm{i}\sin t\ \mathrm{SWAP}. \tag{29}$$

Then with the scaling $t \to 2t$ we obtain $U_{XYZ}(t)$ in agreement with the above expressions.

The symmetric Hamiltonian $H_{XYZ} = H_{XYZ}^T$ gives rise to the symmetric unitary evolution operator $U_{XYZ}(t)$. Then one finds that $\gamma(U_{XYZ}) = U_{XYZ}^2 = \mathrm{e}^{2\mathrm{i}H_{XYZ}t}$. That is, the evolution operator $U_{XYZ}(t)$ and the operator $\gamma[U_{XYZ}(t)]$ are intimately and very simply related by way of $t \to 2t$. This is an instance of the following more general result.

Any symmetric matrix of the form

$$S = \begin{bmatrix} a & 0 & 0 & b \\ 0 & c & s & 0 \\ 0 & s & c & 0 \\ b & 0 & 0 & a \end{bmatrix} \tag{30}$$

is invariant under the transformation $S \to \sigma_y^{\otimes 2} S^T \sigma_y^{\otimes 2}$. Then simply we have $\gamma(S) = S^2$. Such matrices as S will be diagonal in the Bell or magic bases. The evolution operator $U_{XYZ}(t)$ is an example of equation (30) for the special case of $b = 0$.

Additionally of interest for the determination of CNOT gate feasibility, we have from equation (30) for the corresponding characteristic polynomial $\chi[\gamma(S)] = \chi(S^2)$. This polynomial may easily be explicitly written and we omit the details.

The transformation property of S of equation (30) extends to symmetric matrices of the form

$$S = \begin{bmatrix} a & d & e & b \\ d & c & s & -e \\ e & s & c & -d \\ b & -e & -d & a \end{bmatrix}. \tag{31}$$

Then again we have $\gamma(S) = S^2$.

For the important matrix exponentiation problem, still other methods have been given. These include both general [23–25] and specific [26] methods. Putzer [23] gave two methods based upon the fact that $\exp(At)$ is a polynomial in the square matrix A whose coefficients are scalar functions of t. Gantmacher's purely algebraic method [24] is based upon the Lagrange–Sylvester interpolation formula and requires knowing the factorization of the minimal polynomial of A. Another general method was developed by Kirchner [25] using the factorization of the characteristic polynomial of A.

On the other hand, Apostol [26] gave results suited to specific eigenvalue assumptions. In particular, his theorem 2 treats the case of an $n \times n$ matrix A with n distinct eigenvalues λ_k. The result is that

$$\mathrm{e}^{At} = \sum_{k=1}^{n} \mathrm{e}^{\lambda_k t} L_k(A), \tag{32}$$

where the $L_k(A)$ Lagrange interpolation coefficients are given by

$$L_k(A) = \prod_{\substack{j=1 \\ j\neq k}}^{n} \frac{A - \lambda_j I}{\lambda_k - \lambda_j}, \qquad 1 \leqslant k \leqslant n. \tag{33}$$

We may note that separate information on the eigenvectors of A is not required. We describe how this theorem may be extended and briefly illustrate this with respect to an earlier example in the case of $n = 4$.

For matrices of repeated eigenvalues, we may perform the coalescence of eigenvalues in the expressions (32) and (33). We restrict attention here to eigenvalues of multiplicity two and use the limit

$$\lim_{\lambda_j\to\lambda_k}\frac{1}{\lambda_j-\lambda_k}[\mathrm{e}^{\lambda_j t}(A-\lambda_k I)-\mathrm{e}^{\lambda_k t}(A-\lambda_j I)]=[I+(A-\lambda_k I)t]\,\mathrm{e}^{\lambda_k t}, \tag{34}$$

that may be obtained with the aid of L'Hôpital's rule or simply by way of the definition of the derivative with respect to λ_j.

In the case of $n = 4$, omitting details, we find in the case of both $\lambda_1 \to \lambda_2$ and $\lambda_3 \to \lambda_4$ that

$$\mathrm{e}^{At}=\frac{1}{(\lambda_4-\lambda_2)^2}\{(A-\lambda_4 I)^2[(A-\lambda_2 I)t+I]\,\mathrm{e}^{\lambda_2 t}+(A-\lambda_2 I)^2[(A-\lambda_4 I)t+I]\,\mathrm{e}^{\lambda_4 t}\}. \tag{35}$$

In particular, if we now take $\lambda_2 = -\lambda_4$ we are in the same situation as the Hamiltonian H_{bw} with doubly repeated eigenvalues $\pm x$, and equation (35) reduces to previous results.

Extensions to other Hamiltonians

An extension of the above procedures for the determination of CNOT feasibility is to matrices of the form

$$H_{bwv}\equiv\begin{bmatrix} w_1 & 0 & 0 & b_1\\ 0 & w_2 & b_2 & 0\\ 0 & b_2^* & v_2 & 0\\ b_1^* & 0 & 0 & v_1\end{bmatrix}, \tag{36}$$

where w_1, w_2, v_2 and v_1 are real numbers. Again the complex exponentials of these matrices will retain this same form.

The class of matrices of the form of equation (36) includes those of much current interest for superconducting flux qubits [17, 18]. In one method [17] we have the effective Hamiltonian

$$H_{\mathrm{eff}}=\frac{J_{\mathrm{ac}}}{4}[\sigma_z\otimes\sigma_z\pm\sigma_y\otimes\sigma_y], \tag{37}$$

where $J_{\mathrm{ac}} \approx 100$ MHz is the ac coupling energy. Without loss of generality (due to possible scaling) we put

$$H_{\mathrm{eff}}^{(\pm)}=\sigma_z\otimes\sigma_z\pm\sigma_y\otimes\sigma_y=\begin{bmatrix} 1 & 0 & 0 & \mp 1\\ 0 & -1 & \pm 1 & 0\\ 0 & \pm 1 & -1 & 0\\ \mp 1 & 0 & 0 & 1\end{bmatrix}, \tag{38}$$

and $U^{(\pm)}(t) \equiv \exp\big(\mathrm{i}H_{\mathrm{eff}}^{(\pm)}t\big)$. We determine that

$$\gamma(U^{(\pm)})=\frac{1}{2}\begin{bmatrix} 1+\mathrm{e}^{4\mathrm{i}t} & 0 & 0 & \pm(1-\mathrm{e}^{4\mathrm{i}t})\\ 0 & 1+\mathrm{e}^{-4\mathrm{i}t} & \pm(1-\mathrm{e}^{-4\mathrm{i}t}) & 0\\ 0 & \pm(1-\mathrm{e}^{-4\mathrm{i}t}) & 1+\mathrm{e}^{-4\mathrm{i}t} & 0\\ \pm(1-\mathrm{e}^{4\mathrm{i}t}) & 0 & 0 & 1+\mathrm{e}^{4\mathrm{i}t}\end{bmatrix}, \tag{39}$$

and

$$\chi[\gamma(U^{(\pm)})]=(x-1)^2(1-2\cos(4t)x+x^2). \tag{40}$$

Therefore, the evolution operator $U^{(\pm)}$ can be simulated with two CNOT and single-qubit gates.

More generally than equation (37) we may consider Hamiltonians with time-dependent coefficients such as [18]

$$H_{\text{flux}}(t) = -\frac{g_+(t)}{4}(\sigma_x \otimes \sigma_x - \sigma_y \otimes \sigma_y) - \frac{g_-(t)}{4}(\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y). \tag{41}$$

This logical Hamiltonian appears in a design for tunably coupling a pair of flux qubits via the quantum inductance of a third high-frequency qubit. In this setup, all of the time dependence of the Hamiltonian is taken to arise from a time-dependent magnetic flux. Putting $U_{\text{flux}}(t) = \exp\left[\mathrm{i}\int_0^t H_{\text{flux}}(t')\,\mathrm{d}t'\right]$ and $j_\pm(t) = -\int_0^t g_\pm(t')\,\mathrm{d}t'$, we have

$$U_{\text{flux}}(t) = \begin{bmatrix} \cos(j_+/2) & 0 & 0 & \mathrm{i}\sin(j_+/2) \\ 0 & \cos(j_-/2) & \mathrm{i}\sin(j_-/2) & 0 \\ 0 & \mathrm{i}\sin(j_-/2) & \cos(j_-/2) & 0 \\ \mathrm{i}\sin(j_+/2) & 0 & 0 & \cos(j_+/2) \end{bmatrix}. \tag{42}$$

We have $|U_{\text{flux}}| = 1$ and

$$\gamma(U_{\text{flux}}) = \begin{bmatrix} \cos(j_+) & 0 & 0 & \mathrm{i}\sin(j_+) \\ 0 & \cos(j_-) & \mathrm{i}\sin(j_-) & 0 \\ 0 & \mathrm{i}\sin(j_-) & \cos(j_-) & 0 \\ \mathrm{i}\sin(j_+) & 0 & 0 & \cos(j_+) \end{bmatrix}. \tag{43}$$

Furthermore,

$$\chi[\gamma(U_{\text{flux}})] = (1 - 2\cos j_- x + x^2)(1 - 2\cos j_+ x + x^2), \tag{44}$$

so that U_{flux} may be simulated with two CNOT and single-qubit gates in general. When $\cos j_\pm = 0$, we have $\chi[\gamma(U_{\text{flux}})] = (x^2+1)^2$ so U_{flux} is equivalent up to local gates to CNOT. Therefore, U_{flux} may be used to generate a CNOT gate.

Given functions $g_\pm(t) \propto \delta\epsilon_{3\pm}(t)$ where $\delta\epsilon_{3\pm}$ is the amplitude of microwave modulation of the energy level of the third qubit at the sum or difference frequency of the two detuned qubits [18], the time to reach the CNOT gate is given by

$$j_\pm(t) = -\int_0^t g_\pm(t')\,\mathrm{d}t' = \pm(n + 1/2)\pi, \qquad n = 0, 1, 2, \ldots. \tag{45}$$

At say the time $j_\pm/2 = \pi/4$, we have

$$U_{\text{flux}} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 0 & 0 & \mathrm{i} \\ 0 & 1 & \mathrm{i} & 0 \\ 0 & \mathrm{i} & 1 & 0 \\ \mathrm{i} & 0 & 0 & 1 \end{bmatrix}. \tag{46}$$

At such a time this operator maximally entangles the four standard basis states.

Another extension of the above procedure would be to higher dimensional Hamiltonians of special form. These include

$$H_{bw}^{(2^n)} = wI_{2^{n-1}} \otimes \sigma_z + b\sigma_x^{\otimes n}, \tag{47}$$

and

$$H_{XYZ}^{(2^n)} = \sigma_x^{\otimes n} + \sigma_y^{\otimes n} + \sigma_z^{\otimes n}, \tag{48}$$

as well as extensions of equations (36), (38) and (41). The matrix representation of these Hamiltonians still retains a diagonal-plus-cross-diagonal form. As such, their complex exponentials may still be determined by the 2×2 matrix result in equation (7) or by the methods of the previous section. For instance, we have $\left[H_{bw}^{(2^n)}\right]^2 = (w^2+b^2)I_{2^n}$ and $\left[H_{XYZ}^{(2^n)}\right]^2 = 3I_{2^n} + [\mathrm{i}^n + (-\mathrm{i})^n]H_{XYZ}^{(2^n)}$. In the case that $n = 2m$ we have $\left[H_{XYZ}^{(2^n)}\right]^2 = 3I_{2^n} + 2(-1)^m H_{XYZ}^{(2^n)}$. The γ operator extends to $\gamma_n(u) = u\sigma_y^{\otimes n}u^T\sigma_y^{\otimes n}$. However, for $n > 2$, γ_n and $\chi(\gamma_n)$ no longer completely classify the action of a given gate [27]. This aspect is related to the fact that even for $n = 3$ qubits there is no longer a direct analogue of the magic basis as there is for two qubits.

Finally, we note that the Hamiltonians considered in this paper may be efficiently simulated on a quantum computer according to the method of section 4.7.3 of [10] that uses an ancillary qubit (starting and ending in the state $|0\rangle$) and controlled phase shifts based upon tensor products of σ_z interactions. Interactions coming from tensor products of σ_x and σ_y can be replaced in terms of σ_z by appropriate single-qubit gates. In particular, for σ_x interactions we may use the similarity transformation $\sigma_x = R\sigma_z R$, where R is the Hadamard gate, and for σ_y interactions the similarity transformation $\sigma_y = Q\sigma_z Q^\dagger$, where $Q \equiv \frac{1}{\sqrt{2}}\begin{pmatrix} -\mathrm{i} & \mathrm{i} \\ 1 & 1 \end{pmatrix}$. Then it is possible to write the quantum circuit performing the unitary evolution coming from the given Hamiltonian.

Summary

By pursuing an algebraic technique, we have shown how to analytically determine the feasibility of generating a quantum controlled-NOT logic gate from a specified but parameter-dependent two-qubit Hamiltonian. When it is possible for the corresponding evolution operator U to be in the same equivalence class (up to single-qubit gates) as CNOT, we are able to find the necessary evolution time. We thereby generalized some earlier results restricted to numerical investigation [1, 11]. By retaining the parameter dependence in our analytic solution, we are able to show the effect of the corresponding Hamiltonian contribution.

Our method has direct relevance to two-qubit Hamiltonians currently being considered for spin-based and superconductivity-based systems for quantum computing. For spin-based implementations, the exchange interaction is the leading mechanism for realizing two-qubit gates, and strong candidates such as the quantum inductance of an ancillary qubit are emerging for magnetic-flux-based implementations for constructing nonlocal quantum gates. As a particular instance of our results, we showed that the operator U_{flux} of equation (38) is capable of yielding a CNOT gate, with the then concomitant time being given by the condition in equation (41). Our algebraic technique applies to other physical systems for quantum computing, including ion-trap-based systems and optical implementations.

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