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Quantum gate design: A perspective

Michael R. Geller[1,*], Emily J. Pritchett[1], Andrei Galiautdinov[1], and John M. Martinis[2]

[1] Department of Physics and Astronomy, University of Georgia, Athens, Georgia 30602, USA
[2] Department of Physics, University of California, Santa Barbara, California 93106, USA

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* Corresponding author: e-mail mgeller@uga.edu

We give a general discussion of the problem of designing quantum logic gates for physical quantum computing architectures, and explain the use of perturbation theory and the concept of local equivalence.

1 Introduction The problem of quantum gate design can be informally stated as follows: Given a physical Hamiltonian

$$H(\xi_1, \xi_2, \cdots, \xi_K) \tag{1}$$

describing a pair of qubits (understood to be embedded in a large array) with *in-situ* experimental control over parameters $\xi_1, \xi_2, \cdots, \xi_K$, what trajectory of these parameters leads to a desired unitary target? The Hilbert space has to be specified of course, and if we let N be its dimension, we have a control problem in U(N). N isn't necessarily equal to 4 because sometimes it is convenient to use "non-qubit" states, i.e., states that are not in the computational basis

$$\{\langle|00\rangle, |01\rangle, |10\rangle, |11\rangle\}, \tag{2}$$

to help implement the gate, but the U(4) case, where the Hamiltonian can be written in terms of Pauli matrices and their tensor products, will still have wide application. Examples where non-qubit states are used include the anticrossing of the computational $|11\rangle$ manifold with a non-qubit state to generate a CZ gate [1], as well as the approach by Cirac and Zoller [2] to use ionic vibrational modes to implement a CNOT gate for trapped ions.

The gate design problem can be regarded as an inverse problem, where the forward or easy direction is the integration of

$$\dot{U} = -iH\big(\xi_1(t), \xi_2(t), \cdots, \xi_K(t)\big)\, U \tag{3}$$

with initial condition $U(0) = I$. There will be many solutions to the inverse problem, so we have to pick the "best" one according to some criteria. For example, we will often want to find a fast solution (see, for example, Khaneja *et al.* [3]), but experimental simplicity and robustness (weak sensitivity to control errors) are also important.

In the U(4) case the qubit-qubit interaction (in the basis of eigenstates of uncoupled qubits) takes the form

$$\delta H \equiv \sum_{\mu,\nu=x,y,z} J_{\mu\nu}\, \sigma_1^\mu \otimes \sigma_2^\nu \tag{4}$$

with $J_{\mu\nu}$ a real-valued 3×3 tensor. Important special cases of this include the Heisenberg interaction $\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$, the XY interaction $\sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y$, and the Ising interaction $\sigma_1^z\sigma_2^z$. The problem of constructing a CNOT gate in the Heisenberg case, relevant for exchange-coupled electron spins, was solved by Burkard *et al.* [4], and the Ising case is known from NMR quantum computation [5]. However, many architectures being considered for quantum computation involve qubits or qubits and resonators coupled by more complicated and less symmetric interactions. Below we will give a (perturbative) CNOT construction for the general case (4).

We have defined the gate design problem above assuming unitary evolution. Decoherence is of course present in real physical implementations, yet it is still often convenient to separate the fidelity loss caused by decoherence from the *intrinsic* fidelity loss resulting from our failure to reach the target $U_{\rm target}$ exactly, because of errors introduced by approximations such as perturbation theory (see below). Other approaches, such as that of Refs. [6] and [7] include decoherence at the outset, but require knowledge of an accurate decoherence model.

2 Perturbation theory One very important gate design tool is perturbation theory, which also includes approximations such as the RWA. In a wide variety of physical implementations the magnitude of the local single-qubit control fields or the qubit-qubit interaction are small compared with the typical qubit frequency, allowing the Hamiltonian to be simplified (often after transforming to a different representation). By construction, perturbation theory will lead to gates that are slow in real terms (compared to, say, nonperturbative designs with the same fidelity), but they are simple and intuitive, and are likely to be very robust.

A wide variety of weakly coupled and rf-driven qubits can be modeled by a Hamiltonian

$$H = \sum_{i=1,2} \left(-\frac{\epsilon_i}{2}\,\sigma_i^z\right) + \Omega(t)\cos(\epsilon_1 t)\,\sigma_1^x + \delta H, \qquad (5)$$

with δH given in (4). The Hamiltonian (5) is written in the basis of eigenstates of uncoupled qubits with energy level spacings ϵ_i. The ϵ_i are assumed to be experimentally tunable. We have also included resonant rf control of qubit 1 with time-varying amplitude Ω (this will be sufficient for what follows). The magnitude of the elements of $J_{\mu\nu}$ are assumed to be small compared with the ϵ_i. In a frame rotating with the tuned qubits, the Hamiltonian reduces to

$$H \approx \frac{\Omega(t)}{2}\sigma_1^x + \mathcal{H}, \qquad (6)$$

where

$$\mathcal{H} \equiv J\left(\sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y\right) + J_{zz}\,\sigma_1^z\sigma_2^z + J'\left(\sigma_1^x\sigma_2^y - \sigma_1^y\sigma_2^x\right). \qquad (7)$$

Here

$$J \equiv \frac{J_{xx}+J_{yy}}{2} \quad \text{and} \quad J' \equiv \frac{J_{xy}-J_{yx}}{2}. \qquad (8)$$

In the computational basis,

$$\mathcal{H} = \begin{pmatrix} J_{zz} & 0 & 0 & 0 \\ 0 & -J_{zz} & \gamma & 0 \\ 0 & \gamma^* & -J_{zz} & 0 \\ 0 & 0 & 0 & J_{zz} \end{pmatrix}, \quad \gamma \equiv 2(J + iJ'). \qquad (9)$$

To obtain (6) we have assumed that both $J_{\mu\nu}$ and Ω are small compared with the qubit frequency, and we have neglected the resulting rapidly oscillating terms with vanishing time-averages (the this is the usual rotating-wave approximation). Of the 9 coupling constants in δH, only 3 remain in $\mathcal{H}$, making a general analysis possible. The first two terms in (7) are symmetric under qubit-label exchange, whereas the third term is qubit-antisymmetric and vanishes when the qubit devices in question are identical (for example, when applied to a pair of identical superconducting flux qubits).

3 Local equivalence Another powerful design tool is the concept of local equivalence [8,9]. Restricting our discussion to the case of U(4), we face the challenge of steering to a single point in the 16-dimensional group manifold, or a 15-dimensional manifold if we consider SU(4). This problem is vastly simplified in the common limit where independent single-qubit operations

$$u \in \mathrm{SU}(2)_1 \otimes \mathrm{SU}(2)_2 \qquad (10)$$

are fast and accurate, in which case any element in the "local" equivalence class

$$\left\{u_{\mathrm{post}}\,U_{\mathrm{target}}\,u_{\mathrm{pre}}\right\}_{\text{all } u_{\mathrm{pre}} \text{ and } u_{\mathrm{post}}} \qquad (11)$$

will be just as effective as U_{target}. The problem of gate design is now reduced to steering the system to any member of the equivalence class (11) of the desired target.

Makhlin [8] has constructed an explicit formula for 3 quantities that are invariant under the pre- and post-application of arbitrary $\mathrm{SU}(2)_1 \otimes \mathrm{SU}(2)_2$ operations, which can therefore be used to characterize the space of all possible local equivalence classes of U(4). Two members U and U' of U(4) are locally equivalent—related by local rotations—if and only if their Makhlin invariants are identical, in which case we write $U \sim U'$.

Zhang *et al.* [9] have provided a powerful reformulation of the local equivalence concept by using what amounts to a "representation theorem" for U(4), which says that any element can be written as

$$U = e^{i\phi}\,u_{\mathrm{post}}\,e^{-\frac{i}{2}(x\,\sigma_1^x\sigma_2^x + y\,\sigma_1^y\sigma_2^y + z\,\sigma_1^z\sigma_2^z)}\,u_{\mathrm{pre}}, \qquad (12)$$

for some local $\mathrm{SU}(2)_1 \otimes \mathrm{SU}(2)_2$ rotations u_{pre} and u_{pre}, real-valued parameters x, y, and z, and some phase ϕ. This formula can be derived by using a Cartan decomposition of the Lie algebra su(4), the algebra of the generators of the unitary group. The central component

$$U_{\mathrm{ent}} \equiv e^{-\frac{i}{2}(x\,\sigma_1^x\sigma_2^x + y\,\sigma_1^y\sigma_2^y + z\,\sigma_1^z\sigma_2^z)} \qquad (13)$$

in (12), which has the geometrical structure of a 3-torus, evidently characterizes the nonlocal or entangling part of the operation. When restricted to a certain (almost) tetrahedral region—a Weyl chamber—the angles x, y, and z are in one-to-one correspondence with the Makhlin invariants, leading to a beautiful geometric classification of the local equivalence classes.

4 CNOT with weakly coupled qubits In unpublished work we have used perturbation theory and the concept of local equivalence to design a CNOT gate for weakly but otherwise arbitrarily coupled qubits with interaction (4). Zhang and Whaley [10] have also addressed the general problem of two-qubit gate construction using similar methods applied to a variety of coupled-qubit models, but focused on steering with continuous rf control. One of us

has also previously investigated steering with constant applied rf [11,12].

The complete pulse sequence we derive is

$$\mathrm{CNOT} = e^{i(\frac{3\pi}{4})} R_z\big(\tfrac{\pi}{2}\big)_1 R_y\big(-\tfrac{\pi}{2}\big)_1 R_x\big(-\tfrac{\pi}{2}\big)_2 \times R_z\big(-\varphi\big)_2 U_{\mathrm{int}} R_x\big(\pi\big)_1 U_{\mathrm{int}} R_z\big(\varphi\big)_2 R_y\big(\tfrac{\pi}{2}\big)_1 \quad (14)$$

where

$$U_{\mathrm{int}} \equiv e^{-i\mathcal{H}\,\Delta t}, \quad (15)$$

with

$$\Delta t \equiv \frac{\pi}{8\sqrt{J^2 + J'^2}}. \quad (16)$$

Here $R_\mu(\theta)_i \equiv e^{-i(\theta/2)\sigma_i^\mu}$ is a μ rotation on qubit i. $\varphi \equiv \arg\gamma$ is the phase of the complex matrix element γ defined in (9), and we note that apart from these z rotations, the local rotations needed to obtain the CNOT are independent of the parameters J, J_{zz}, and J' characterizing the Hamiltonian $\mathcal{H}$. The construction (14) is simple to implement and applies to a wide variety of coupled qubit models.

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